



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 9PC6 / pdb\_00009pc6  
EMDB ID : EMD-71497  
Title : Antibody (1B2) Bound Crosslinked Rifamycin Synthetase Module 1 with a C-terminal Type II Thioesterase  
Authors : Cogan, D.P.; Liu, C.; West, R.C.; Chen, M.  
Deposited on : 2025-06-27  
Resolution : 3.96 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

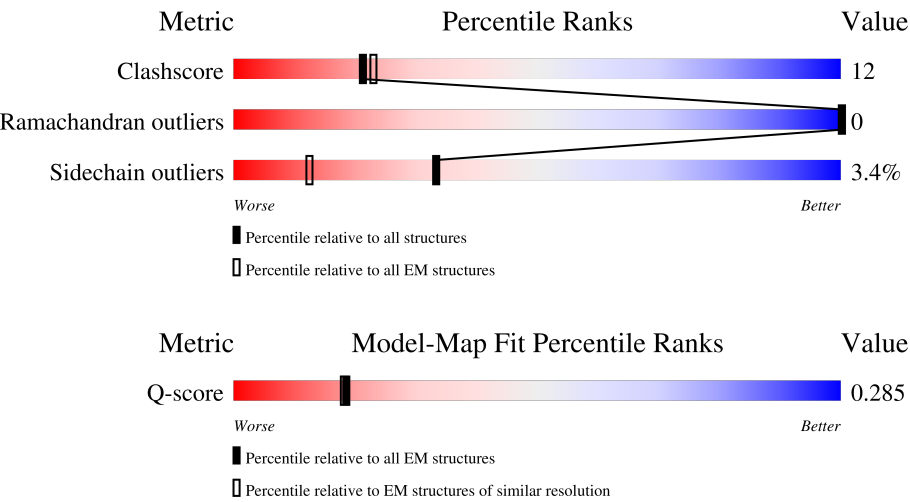
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7646 ( 3.46 - 4.46 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1869	<div><div>26%</div><div>60%</div><div>24%</div><div>16%</div></div>
1	B	1869	<div><div>25%</div><div>62%</div><div>21%</div><div>16%</div></div>
2	J	249	<div><div>14%</div><div>60%</div><div>22%</div><div>18%</div></div>
2	K	249	<div><div>13%</div><div>61%</div><div>20%</div><div>18%</div></div>

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Mol	Chain	Length	Quality of chain
3	I	236	<div><div></div><div>11%</div><div>61%</div><div>26%</div><div>•</div><div>11%</div></div>
3	L	236	<div><div></div><div>10%</div><div>66%</div><div>21%</div><div>•</div><div>11%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29408 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6-deoxyerythronolide-B synthase,RifR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1576	Total	C	N	O	P	S	0	0
			11580	7228	2093	2231	1	27		
1	B	1573	Total	C	N	O	P	S	0	0
			11558	7216	2090	2224	1	27		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O54666
A	2	ALA	-	expression tag	UNP O54666
A	3	SER	-	expression tag	UNP O54666
A	4	THR	-	expression tag	UNP O54666
A	5	ASP	-	expression tag	UNP O54666
A	6	SER	-	expression tag	UNP O54666
A	7	GLU	-	expression tag	UNP O54666
A	8	LYS	-	expression tag	UNP O54666
A	9	VAL	-	expression tag	UNP O54666
A	10	ALA	-	expression tag	UNP O54666
A	11	GLU	-	expression tag	UNP O54666
A	12	TYR	-	expression tag	UNP O54666
A	13	LEU	-	expression tag	UNP O54666
A	14	ARG	-	expression tag	UNP O54666
A	15	ARG	-	expression tag	UNP O54666
A	16	ALA	-	expression tag	UNP O54666
A	17	THR	-	expression tag	UNP O54666
A	18	LEU	-	expression tag	UNP O54666
A	19	ASP	-	expression tag	UNP O54666
A	20	LEU	-	expression tag	UNP O54666
A	21	ARG	-	expression tag	UNP O54666
A	22	ALA	-	expression tag	UNP O54666
A	23	ALA	-	expression tag	UNP O54666
A	24	ARG	-	expression tag	UNP O54666
A	25	GLN	-	expression tag	UNP O54666
A	26	ARG	-	expression tag	UNP O54666

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ILE	-	expression tag	UNP O54666
A	28	ARG	-	expression tag	UNP O54666
A	29	GLU	-	expression tag	UNP O54666
A	30	LEU	-	expression tag	UNP O54666
A	31	GLU	-	expression tag	UNP O54666
A	1582	GLY	-	linker	UNP O54666
A	1583	GLY	-	linker	UNP O54666
A	1584	GLY	-	linker	UNP O54666
A	1585	GLY	-	linker	UNP O54666
A	1586	SER	-	linker	UNP O54666
A	1587	GLY	-	linker	UNP O54666
A	1588	GLY	-	linker	UNP O54666
A	1589	GLY	-	linker	UNP O54666
A	1590	GLY	-	linker	UNP O54666
A	1591	SER	-	linker	UNP O54666
A	1850	GLY	-	expression tag	UNP Q7BUF9
A	1851	ASN	-	expression tag	UNP Q7BUF9
A	1852	SER	-	expression tag	UNP Q7BUF9
A	1853	SER	-	expression tag	UNP Q7BUF9
A	1854	SER	-	expression tag	UNP Q7BUF9
A	1855	VAL	-	expression tag	UNP Q7BUF9
A	1856	ASP	-	expression tag	UNP Q7BUF9
A	1857	LYS	-	expression tag	UNP Q7BUF9
A	1858	LEU	-	expression tag	UNP Q7BUF9
A	1859	ALA	-	expression tag	UNP Q7BUF9
A	1860	ALA	-	expression tag	UNP Q7BUF9
A	1861	ALA	-	expression tag	UNP Q7BUF9
A	1862	LEU	-	expression tag	UNP Q7BUF9
A	1863	GLU	-	expression tag	UNP Q7BUF9
A	1864	HIS	-	expression tag	UNP Q7BUF9
A	1865	HIS	-	expression tag	UNP Q7BUF9
A	1866	HIS	-	expression tag	UNP Q7BUF9
A	1867	HIS	-	expression tag	UNP Q7BUF9
A	1868	HIS	-	expression tag	UNP Q7BUF9
A	1869	HIS	-	expression tag	UNP Q7BUF9
B	1	MET	-	expression tag	UNP O54666
B	2	ALA	-	expression tag	UNP O54666
B	3	SER	-	expression tag	UNP O54666
B	4	THR	-	expression tag	UNP O54666
B	5	ASP	-	expression tag	UNP O54666
B	6	SER	-	expression tag	UNP O54666
B	7	GLU	-	expression tag	UNP O54666

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LYS	-	expression tag	UNP O54666
B	9	VAL	-	expression tag	UNP O54666
B	10	ALA	-	expression tag	UNP O54666
B	11	GLU	-	expression tag	UNP O54666
B	12	TYR	-	expression tag	UNP O54666
B	13	LEU	-	expression tag	UNP O54666
B	14	ARG	-	expression tag	UNP O54666
B	15	ARG	-	expression tag	UNP O54666
B	16	ALA	-	expression tag	UNP O54666
B	17	THR	-	expression tag	UNP O54666
B	18	LEU	-	expression tag	UNP O54666
B	19	ASP	-	expression tag	UNP O54666
B	20	LEU	-	expression tag	UNP O54666
B	21	ARG	-	expression tag	UNP O54666
B	22	ALA	-	expression tag	UNP O54666
B	23	ALA	-	expression tag	UNP O54666
B	24	ARG	-	expression tag	UNP O54666
B	25	GLN	-	expression tag	UNP O54666
B	26	ARG	-	expression tag	UNP O54666
B	27	ILE	-	expression tag	UNP O54666
B	28	ARG	-	expression tag	UNP O54666
B	29	GLU	-	expression tag	UNP O54666
B	30	LEU	-	expression tag	UNP O54666
B	31	GLU	-	expression tag	UNP O54666
B	1582	GLY	-	linker	UNP O54666
B	1583	GLY	-	linker	UNP O54666
B	1584	GLY	-	linker	UNP O54666
B	1585	GLY	-	linker	UNP O54666
B	1586	SER	-	linker	UNP O54666
B	1587	GLY	-	linker	UNP O54666
B	1588	GLY	-	linker	UNP O54666
B	1589	GLY	-	linker	UNP O54666
B	1590	GLY	-	linker	UNP O54666
B	1591	SER	-	linker	UNP O54666
B	1850	GLY	-	expression tag	UNP Q7BUF9
B	1851	ASN	-	expression tag	UNP Q7BUF9
B	1852	SER	-	expression tag	UNP Q7BUF9
B	1853	SER	-	expression tag	UNP Q7BUF9
B	1854	SER	-	expression tag	UNP Q7BUF9
B	1855	VAL	-	expression tag	UNP Q7BUF9
B	1856	ASP	-	expression tag	UNP Q7BUF9
B	1857	LYS	-	expression tag	UNP Q7BUF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1858	LEU	-	expression tag	UNP Q7BUF9
B	1859	ALA	-	expression tag	UNP Q7BUF9
B	1860	ALA	-	expression tag	UNP Q7BUF9
B	1861	ALA	-	expression tag	UNP Q7BUF9
B	1862	LEU	-	expression tag	UNP Q7BUF9
B	1863	GLU	-	expression tag	UNP Q7BUF9
B	1864	HIS	-	expression tag	UNP Q7BUF9
B	1865	HIS	-	expression tag	UNP Q7BUF9
B	1866	HIS	-	expression tag	UNP Q7BUF9
B	1867	HIS	-	expression tag	UNP Q7BUF9
B	1868	HIS	-	expression tag	UNP Q7BUF9
B	1869	HIS	-	expression tag	UNP Q7BUF9

- Molecule 2 is a protein called Antibody Fragment 1B2 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	K	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

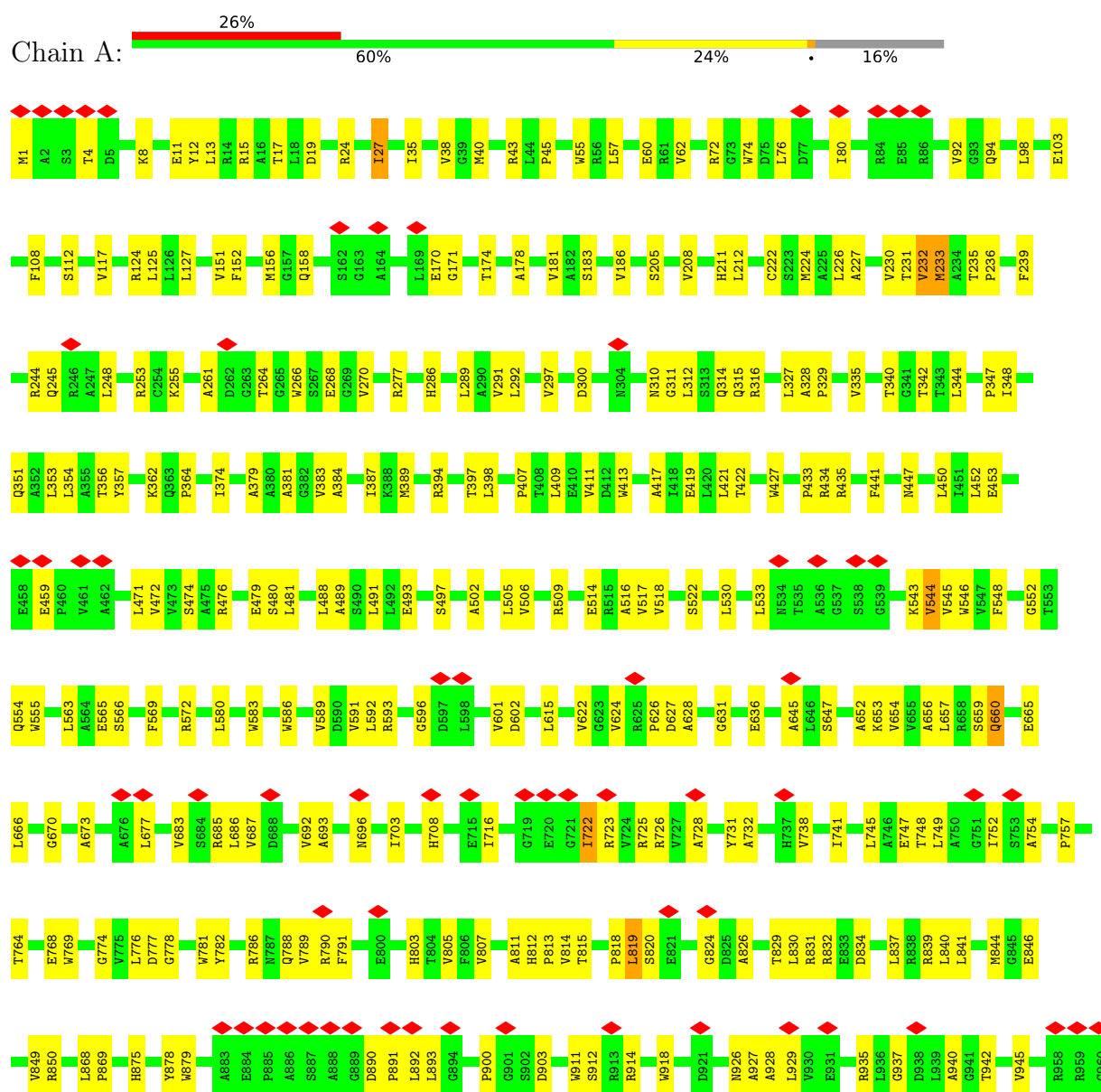
- Molecule 3 is a protein called Antibody Fragment 1B2 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	209	Total	C	N	O	S	0	0
			1596	1001	269	320	6		
3	L	209	Total	C	N	O	S	0	0
			1596	1001	269	320	6		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 6-deoxyerythronolide-B synthase,RifR

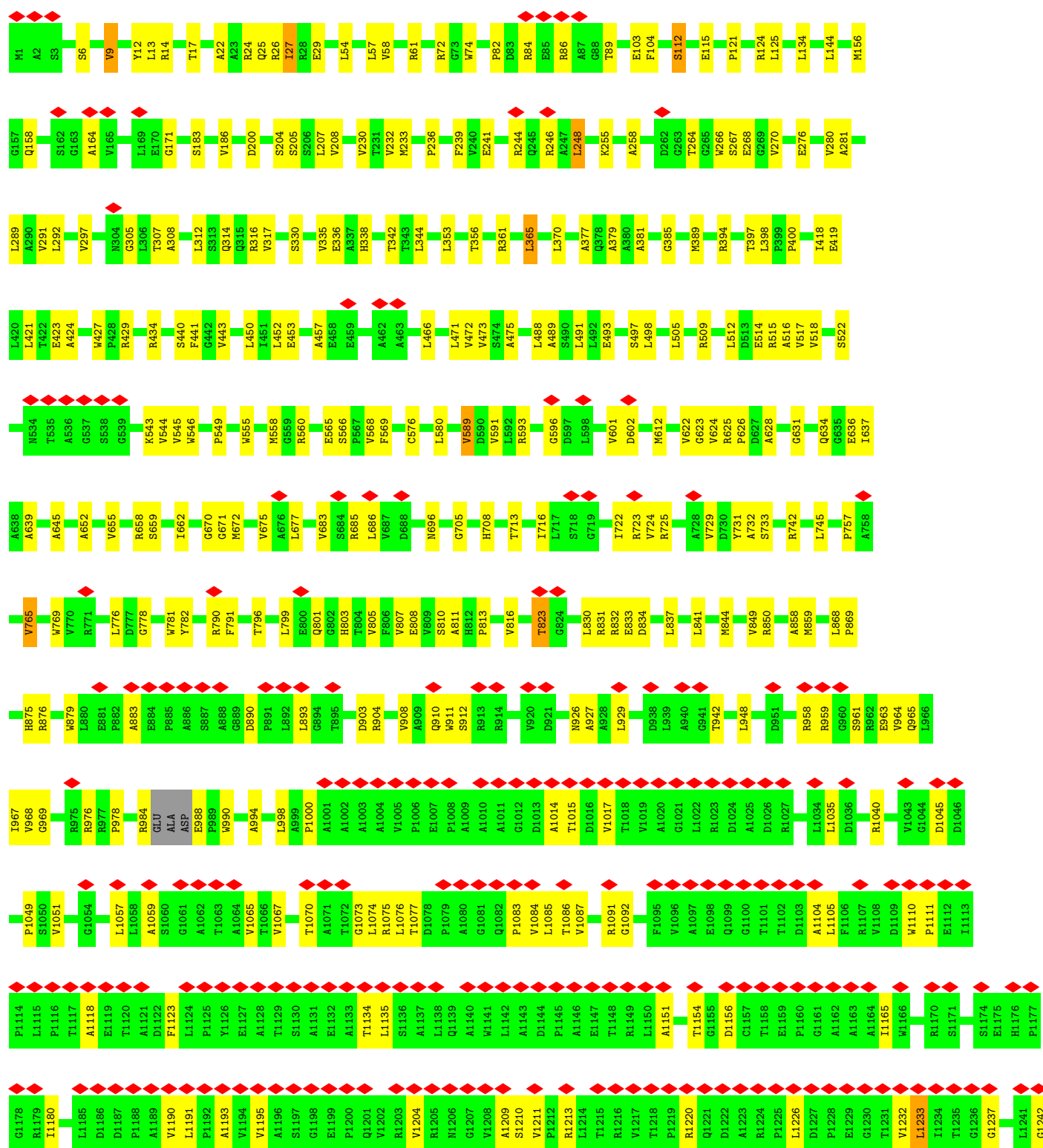


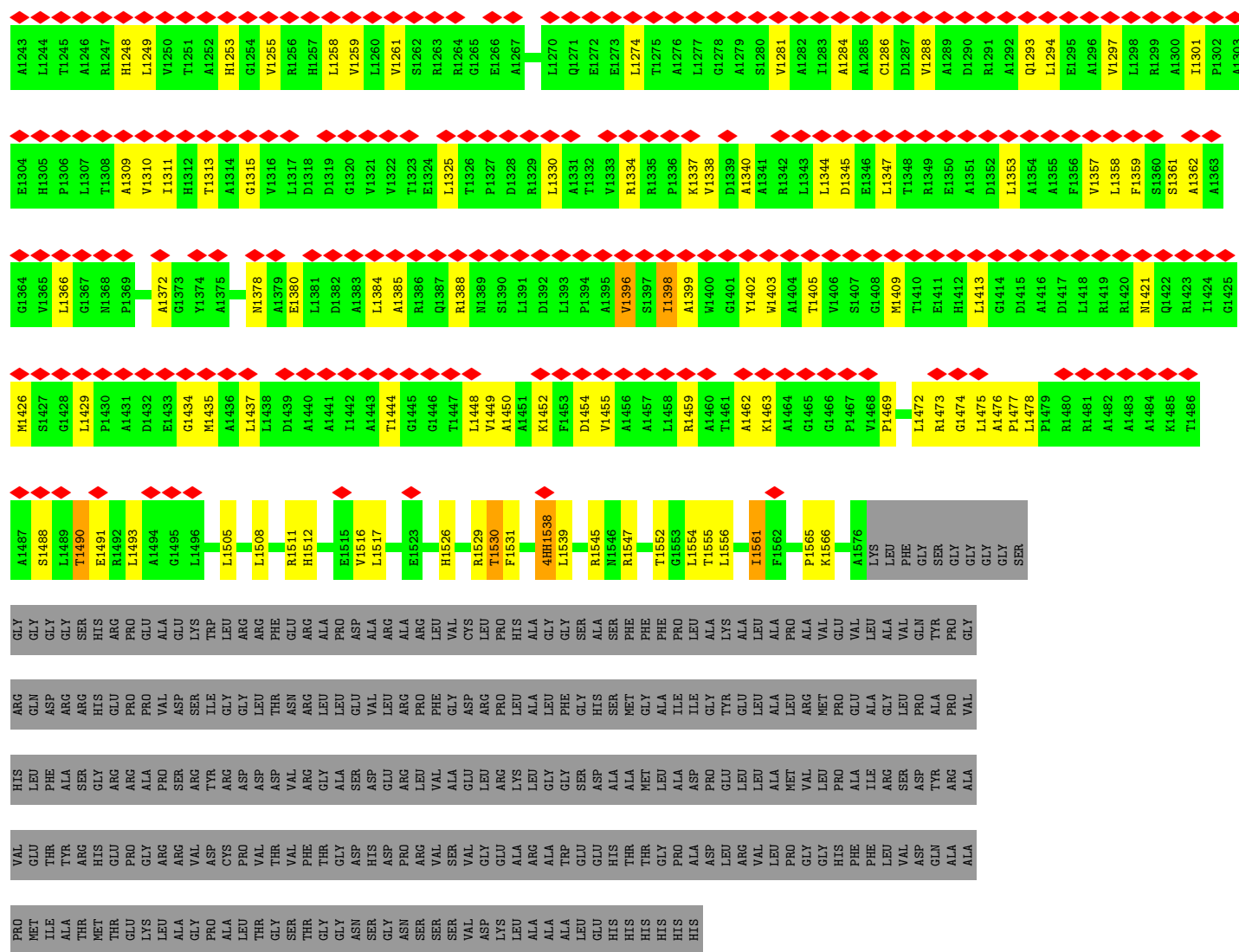




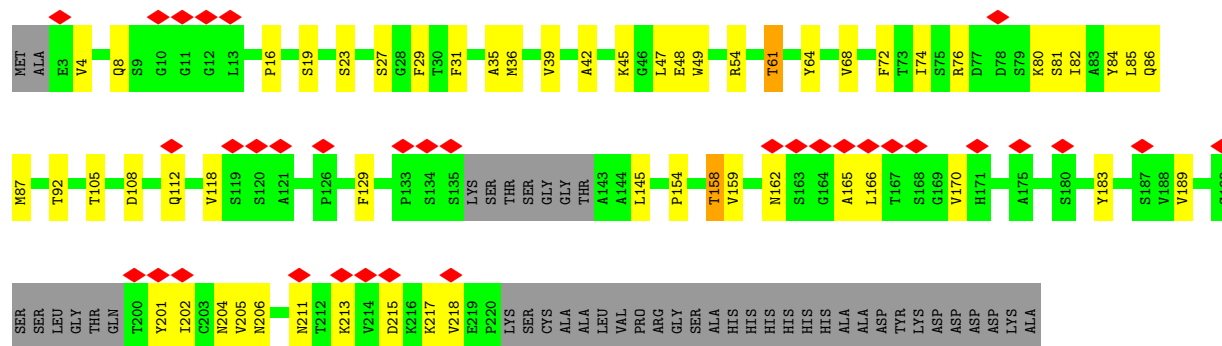
GLY
ASN
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GLY
ASN
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SER
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ASP
LYS
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• Molecule 1: 6-deoxyerythronolide-B synthase,RifR



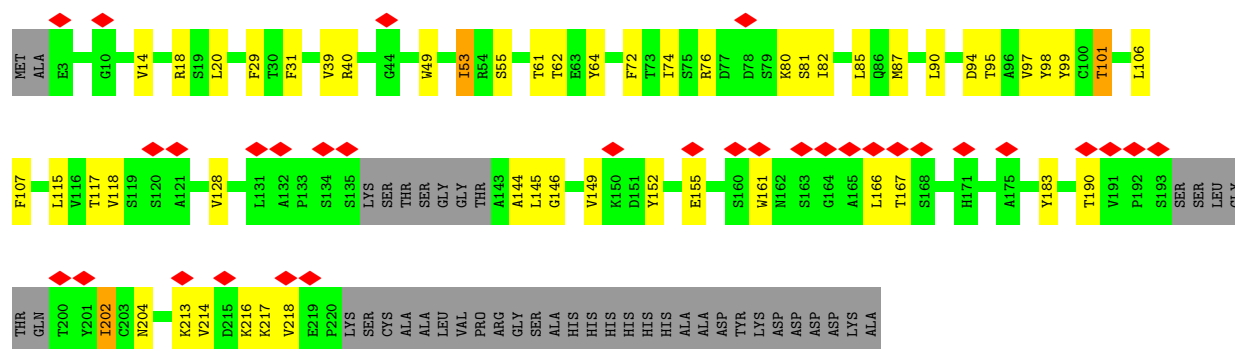


### • Molecule 2: Antibody Fragment 1B2 Heavy Chain

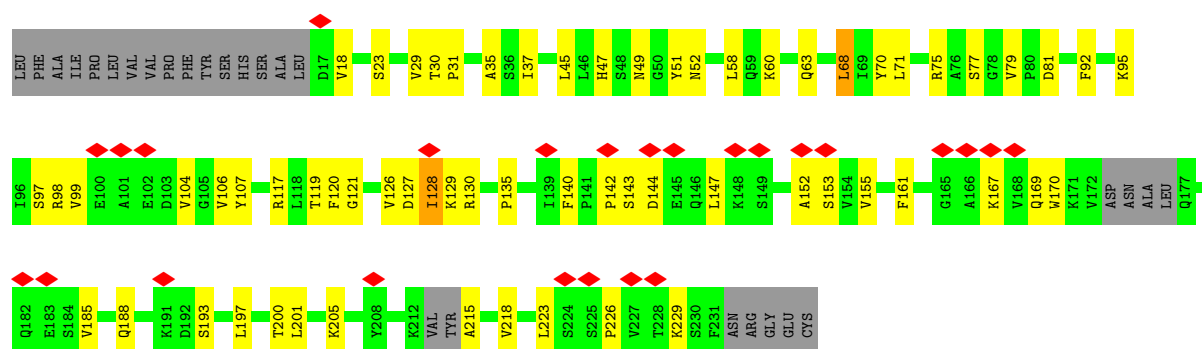


### • Molecule 2: Antibody Fragment 1B2 Heavy Chain

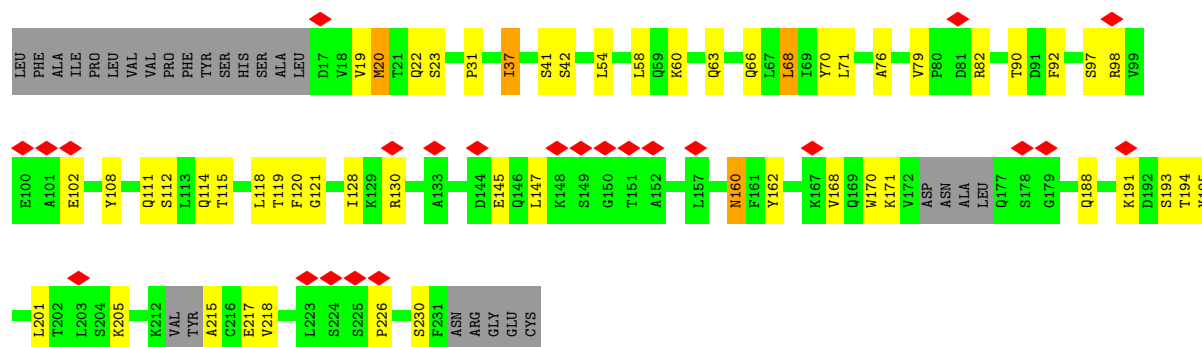




• Molecule 3: Antibody Fragment 1B2 Light Chain



• Molecule 3: Antibody Fragment 1B2 Light Chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3677	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0502	Depositor
Map size (Å)	438.0, 438.0, 438.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.12	0/11769	0.31	0/16083
1	B	0.11	0/11746	0.29	0/16050
2	J	0.12	0/1575	0.34	0/2141
2	K	0.11	0/1575	0.28	0/2141
3	I	0.11	0/1630	0.31	0/2212
3	L	0.19	0/1630	0.36	0/2212
All	All	0.12	0/29925	0.31	0/40839

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11580	0	11559	297	0
1	B	11558	0	11543	257	0
2	J	1539	0	1513	43	0
2	K	1539	0	1513	37	0
3	I	1596	0	1561	43	0
3	L	1596	0	1561	36	0
All	All	29408	0	29250	689	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (689) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:ALA:HA	1:B:1067:VAL:O	1.67	0.93
2:J:85:LEU:HG	2:J:87:MET:HE1	1.62	0.80
1:A:35:ILE:HG22	1:A:292:LEU:HB2	1.64	0.79
1:B:685:ARG:HH21	1:B:716:ILE:HB	1.48	0.79
1:B:233:MET:HE1	1:B:266:TRP:HB3	1.66	0.78
1:A:692:VAL:HA	1:A:703:ILE:HG22	1.67	0.77
1:A:1073:GLY:HA3	1:A:1087:VAL:O	1.85	0.76
1:A:171:GLY:HA3	1:B:244:ARG:HH22	1.49	0.76
3:I:31:PRO:HD3	3:I:128:ILE:HD11	1.67	0.74
3:I:51:TYR:HB3	3:I:71:LEU:HD11	1.70	0.73
1:A:328:ALA:HB2	3:L:98:ARG:HH12	1.52	0.73
1:A:1396:VAL:HG21	1:A:1441:ALA:HB1	1.70	0.72
1:B:1399:ALA:HB3	1:B:1449:VAL:HG22	1.73	0.71
1:B:1338:VAL:HG13	1:B:1384:LEU:HD11	1.72	0.71
1:B:976:ARG:HA	1:B:998:LEU:O	1.91	0.71
2:J:159:VAL:HG22	2:J:205:VAL:HG13	1.73	0.71
1:A:1400:TRP:HH2	1:A:1438:LEU:HB2	1.56	0.71
1:B:670:GLY:HA3	1:B:732:ALA:HB2	1.73	0.71
1:A:1043:VAL:HG21	1:A:1049:PRO:HB3	1.73	0.70
3:L:130:ARG:HD2	3:L:193:SER:HB2	1.73	0.70
1:A:124:ARG:HA	1:A:127:LEU:HD12	1.74	0.70
1:A:1135:LEU:HD22	1:A:1330:LEU:HD11	1.72	0.70
1:A:544:VAL:HG13	1:A:627:ASP:H	1.57	0.70
1:B:543:LYS:HB2	1:B:803:HIS:HA	1.73	0.70
1:B:156:MET:HE1	1:B:200:ASP:HB2	1.73	0.69
1:A:398:LEU:HB3	1:A:421:LEU:HD21	1.73	0.69
1:A:170:GLU:HG2	1:B:244:ARG:NH1	2.06	0.69
1:A:103:GLU:HB3	1:A:875:HIS:HB3	1.74	0.69
1:A:693:ALA:H	1:A:703:ILE:HA	1.58	0.69
1:B:612:MET:HE1	1:B:810:SER:HA	1.74	0.69
1:B:685:ARG:HH22	1:B:713:THR:HA	1.58	0.69
1:A:340:THR:HG23	1:A:342:THR:H	1.59	0.68
3:I:142:PRO:HB3	3:I:153:SER:H	1.58	0.68
1:B:1057:LEU:HD13	1:B:1085:LEU:HD12	1.75	0.68
2:J:39:VAL:HG22	2:J:49:TRP:HA	1.75	0.68
1:A:471:LEU:HD12	1:A:505:LEU:HD21	1.74	0.68
1:A:40:MET:HE1	1:A:387:ILE:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:HB2	1:B:1517:LEU:HG	1.75	0.68
2:K:145:LEU:HD12	2:K:218:VAL:HB	1.76	0.68
1:B:683:VAL:HA	1:B:686:LEU:HD23	1.76	0.67
1:A:1458:LEU:HB3	1:A:1476:ALA:HB2	1.75	0.67
1:A:591:VAL:HG12	1:A:596:GLY:HA3	1.77	0.67
1:A:1346:GLU:HA	1:A:1349:ARG:HD2	1.76	0.67
1:A:1517:LEU:HB2	1:A:1519:HIS:HD2	1.60	0.67
1:A:677:LEU:HD21	1:A:722:ILE:HG21	1.76	0.66
1:A:1237:GLY:HA3	1:A:1260:LEU:HB3	1.75	0.66
2:K:87:MET:HG2	2:K:90:LEU:HD21	1.77	0.66
1:A:545:VAL:HG22	1:A:628:ALA:HB3	1.76	0.66
1:B:799:LEU:HD11	1:B:823:THR:HG22	1.76	0.66
1:B:475:ALA:O	1:B:514:GLU:HB2	1.95	0.66
1:B:832:ARG:HG2	1:B:833:GLU:HG3	1.77	0.66
1:B:471:LEU:HD12	1:B:505:LEU:HD21	1.76	0.66
1:A:657:LEU:HD13	1:A:748:THR:HB	1.78	0.66
1:A:1151:ALA:HB1	1:A:1191:LEU:HD11	1.77	0.66
1:A:831:ARG:HB2	1:A:839:ARG:HE	1.60	0.65
2:J:74:ILE:HG23	2:J:85:LEU:HD13	1.76	0.65
1:B:291:VAL:HG23	1:B:453:GLU:HB3	1.79	0.65
1:A:1105:LEU:HD13	1:A:1448:LEU:HD13	1.78	0.65
1:A:233:MET:HE1	1:A:266:TRP:HB3	1.77	0.64
1:B:12:TYR:HE2	3:L:71:LEU:HG	1.62	0.64
1:A:890:ASP:HB2	1:A:935:ARG:HH21	1.63	0.64
1:B:1258:LEU:HB2	1:B:1281:VAL:HG22	1.79	0.64
1:A:602:ASP:HA	1:A:659:SER:HB2	1.79	0.64
3:L:70:TYR:HD1	3:L:71:LEU:HD12	1.62	0.64
1:B:545:VAL:HG22	1:B:628:ALA:HB3	1.79	0.64
1:B:637:ILE:HD13	1:B:655:VAL:HB	1.79	0.63
3:L:19:VAL:HG12	3:L:41:SER:HB2	1.78	0.63
1:B:723:ARG:HH22	1:B:725:ARG:HD3	1.63	0.63
3:L:168:VAL:HG22	3:L:218:VAL:HG22	1.80	0.63
1:A:1473:ARG:HH21	1:A:1478:LEU:H	1.46	0.63
1:A:43:ARG:HB2	1:A:270:VAL:HB	1.80	0.63
1:A:409:LEU:HD23	1:A:409:LEU:H	1.61	0.63
1:B:602:ASP:HA	1:B:659:SER:HB2	1.81	0.63
1:B:312:LEU:HB3	1:B:316:ARG:HH12	1.62	0.63
1:A:552:GLY:H	1:A:554:GLN:HE22	1.47	0.63
2:K:128:VAL:HG12	2:K:149:VAL:HG12	1.81	0.63
2:K:55:SER:HA	2:K:76:ARG:HH22	1.64	0.62
1:B:1059:ALA:HB3	1:B:1084:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:HG22	1:B:344:LEU:H	1.62	0.62
1:A:156:MET:HE1	1:A:379:ALA:HB2	1.81	0.62
1:A:208:VAL:HG23	1:A:297:VAL:HG21	1.81	0.62
1:B:1402:TYR:HB2	1:B:1413:LEU:HD11	1.82	0.62
1:A:1512:HIS:O	1:A:1516:VAL:HG23	2.00	0.61
1:B:398:LEU:HB3	1:B:421:LEU:HD21	1.82	0.61
1:A:158:GLN:HE22	1:A:235:THR:H	1.48	0.61
1:B:1073:GLY:HA3	1:B:1087:VAL:O	2.00	0.61
1:B:1530:THR:HB	1:B:1565:PRO:HB2	1.83	0.61
1:A:723:ARG:HH12	1:A:725:ARG:HB2	1.66	0.60
1:A:230:VAL:HG12	1:A:270:VAL:HG13	1.83	0.60
1:B:984:ARG:HB2	1:B:988:GLU:HG2	1.83	0.60
1:B:1151:ALA:HB1	1:B:1191:LEU:HD11	1.83	0.60
1:B:1261:VAL:HG12	1:B:1284:ALA:HB3	1.83	0.60
1:B:1259:VAL:HG21	1:B:1301:ILE:HG12	1.81	0.60
1:B:389:MET:HE3	1:B:389:MET:HA	1.82	0.60
1:B:645:ALA:HB2	1:B:757:PRO:HB3	1.83	0.60
1:B:1274:LEU:HD13	1:B:1281:VAL:HG21	1.84	0.60
1:A:239:PHE:HE1	1:A:266:TRP:HB2	1.66	0.60
1:A:1402:TYR:HB2	1:A:1413:LEU:HD11	1.82	0.60
1:B:103:GLU:HB3	1:B:875:HIS:HB3	1.84	0.60
1:B:338:HIS:CE1	1:B:441:PHE:H	2.20	0.60
1:A:232:VAL:HA	1:A:268:GLU:HG2	1.84	0.60
1:A:543:LYS:HB2	1:A:803:HIS:HA	1.84	0.60
1:A:840:LEU:HG	1:A:844:MET:HE1	1.84	0.60
1:A:891:PRO:HD3	1:A:1027:ARG:HH21	1.67	0.60
1:A:1199:GLU:HG3	1:A:1201:GLN:H	1.65	0.60
2:J:23:SER:HB2	2:J:82:ILE:HD11	1.84	0.59
1:B:672:MET:HE3	1:B:729:VAL:HG11	1.83	0.59
3:I:45:LEU:HD13	3:I:92:PHE:HE1	1.67	0.59
3:L:68:LEU:HA	3:L:79:VAL:HG21	1.82	0.59
1:B:1288:VAL:HG22	1:B:1340:ALA:HB1	1.83	0.59
1:B:1462:ALA:HB2	1:B:1476:ALA:HB1	1.84	0.59
3:L:19:VAL:CG1	3:L:41:SER:HB2	2.32	0.59
3:L:31:PRO:HD3	3:L:128:ILE:HD11	1.84	0.59
1:A:353:LEU:HA	1:A:356:THR:HG22	1.84	0.59
1:A:1107:ARG:HH11	1:A:1447:THR:HB	1.68	0.59
2:J:87:MET:N	2:J:87:MET:HE2	2.17	0.59
1:A:1190:VAL:HG21	1:A:1204:VAL:HG11	1.83	0.59
1:B:472:VAL:HG12	1:B:517:VAL:HG12	1.83	0.59
1:B:1051:VAL:HG11	1:B:1091:ARG:HH21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:VAL:HG21	1:B:1204:VAL:HG11	1.84	0.59
1:A:811:ALA:HA	1:A:830:LEU:HB2	1.84	0.59
1:B:1362:ALA:HB1	1:B:1366:LEU:HD12	1.84	0.59
1:A:1487:ALA:HB1	1:A:1491:GLU:HB2	1.84	0.58
1:B:74:TRP:CD2	1:B:236:PRO:HG3	2.38	0.58
2:J:92:THR:HA	2:J:118:VAL:HB	1.85	0.58
2:K:39:VAL:HG23	2:K:49:TRP:HA	1.84	0.58
1:A:548:PHE:HB2	1:A:631:GLY:HA2	1.84	0.58
1:A:1541:ALA:HA	1:A:1544:LEU:HD23	1.84	0.58
1:B:1261:VAL:HG11	1:B:1297:VAL:HG11	1.84	0.58
1:A:841:LEU:HA	1:A:844:MET:SD	2.43	0.58
1:A:1552:THR:HG23	1:A:1554:LEU:H	1.68	0.58
1:B:230:VAL:HG23	1:B:270:VAL:HB	1.85	0.58
3:I:135:PRO:HD2	3:I:223:LEU:HG	1.84	0.58
1:A:171:GLY:CA	1:B:244:ARG:HH12	2.17	0.58
1:B:927:ALA:HB1	1:B:1035:LEU:HB3	1.86	0.58
3:I:60:LYS:HB2	3:I:63:GLN:HB2	1.86	0.58
1:A:749:LEU:HD13	1:A:781:TRP:HD1	1.67	0.58
1:B:677:LEU:HD11	1:B:722:ILE:HD13	1.86	0.57
1:A:1110:TRP:HB3	1:A:1210:SER:HB2	1.86	0.57
1:B:841:LEU:HA	1:B:844:MET:HE3	1.85	0.57
1:A:502:ALA:O	1:A:506:VAL:HG12	2.05	0.57
1:B:969:GLY:HA3	1:B:978:PRO:HG2	1.86	0.57
1:B:429:ARG:HH12	1:B:457:ALA:HB2	1.70	0.57
1:B:745:LEU:HD11	1:B:782:TYR:HB2	1.87	0.57
1:A:1259:VAL:HG22	1:A:1282:ALA:HB3	1.87	0.57
1:B:1213:ARG:HD2	1:B:1474:GLY:H	1.70	0.57
3:I:218:VAL:O	3:I:226:PRO:HA	2.05	0.56
1:B:1220:ARG:HD2	1:B:1444:THR:HA	1.86	0.56
1:A:601:VAL:HG11	1:A:731:TYR:HE1	1.71	0.56
1:B:560:ARG:HA	1:B:593:ARG:HG2	1.87	0.56
1:A:926:ASN:HA	1:A:929:LEU:HD23	1.87	0.56
2:K:53:ILE:HB	2:K:74:ILE:HD13	1.86	0.56
1:A:1213:ARG:HH21	1:A:1473:ARG:HH11	1.53	0.56
1:B:1313:THR:HA	1:B:1359:PHE:HB2	1.85	0.56
1:B:248:LEU:HA	1:B:264:THR:H	1.71	0.56
1:A:696:ASN:HA	1:A:791:PHE:HB3	1.86	0.56
2:J:170:VAL:HG22	2:J:189:VAL:HG22	1.88	0.55
3:L:23:SER:HB2	3:L:37:ILE:HD11	1.88	0.55
1:A:892:LEU:HA	1:A:911:TRP:HE1	1.70	0.55
1:B:696:ASN:HA	1:B:791:PHE:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1135:LEU:HD22	1:B:1330:LEU:HD11	1.88	0.55
1:A:563:LEU:HD22	1:A:592:LEU:HD11	1.89	0.55
1:A:890:ASP:HB3	1:A:893:LEU:HB2	1.89	0.55
1:A:389:MET:HA	1:A:389:MET:HE3	1.88	0.55
1:A:509:ARG:HH21	1:A:868:LEU:HB2	1.71	0.55
1:B:555:TRP:CE2	1:B:832:ARG:HA	2.42	0.55
1:A:726:ARG:HH21	1:A:728:ALA:HA	1.72	0.55
3:I:142:PRO:HG3	3:I:152:ALA:HB1	1.89	0.55
1:A:19:ASP:OD1	3:I:77:SER:HB2	2.06	0.54
1:A:745:LEU:HD22	1:A:782:TYR:HB2	1.87	0.54
1:A:1385:ALA:HB3	1:A:1397:SER:HB2	1.88	0.54
2:K:95:THR:HG23	2:K:117:THR:HA	1.89	0.54
2:K:202:ILE:HG22	2:K:217:LYS:HG2	1.88	0.54
1:A:1059:ALA:HB3	1:A:1084:VAL:HG13	1.89	0.54
1:B:634:GLN:O	1:B:637:ILE:HG22	2.07	0.54
1:A:1271:GLN:HG3	1:A:1281:VAL:HB	1.89	0.54
1:B:778:GLY:HA2	1:B:781:TRP:CD1	2.42	0.54
1:A:1105:LEU:HD12	1:A:1219:PRO:HG3	1.89	0.54
1:A:1515:GLU:HG2	1:A:1547:ARG:HH22	1.72	0.54
2:K:128:VAL:HG23	2:K:216:LYS:HZ2	1.72	0.54
1:B:208:VAL:HG23	1:B:297:VAL:HG21	1.90	0.54
1:B:558:MET:HA	1:B:558:MET:HE3	1.90	0.54
1:B:1545:ARG:HG3	1:B:1556:LEU:HB2	1.89	0.54
2:J:158:THR:HG23	2:J:206:ASN:HB3	1.89	0.54
1:A:927:ALA:HB1	1:A:1035:LEU:HB3	1.89	0.54
1:A:1359:PHE:HA	1:A:1400:TRP:HE1	1.72	0.54
1:B:580:LEU:HD21	1:B:652:ALA:HB1	1.90	0.54
1:B:742:ARG:HG2	1:B:782:TYR:CZ	2.42	0.54
1:A:312:LEU:HG	1:A:316:ARG:HH12	1.73	0.54
1:B:289:LEU:HD13	1:B:394:ARG:HH22	1.73	0.54
1:B:489:ALA:O	1:B:493:GLU:HG2	2.08	0.54
1:A:982:PHE:HB3	1:A:990:TRP:CE3	2.43	0.53
1:A:1051:VAL:HB	1:A:1091:ARG:HB2	1.89	0.53
1:A:1358:LEU:HD12	1:A:1385:ALA:HB2	1.90	0.53
1:B:1065:VAL:HG21	1:B:1076:LEU:HB3	1.90	0.53
1:B:6:SER:HA	1:B:9:VAL:HB	1.90	0.53
1:B:1075:ARG:HG2	1:B:1086:THR:HG22	1.90	0.53
2:J:42:ALA:HB3	2:J:45:LYS:HB2	1.91	0.53
2:J:72:PHE:HB3	2:J:85:LEU:HD11	1.90	0.53
1:A:74:TRP:CD2	1:A:236:PRO:HG3	2.43	0.53
1:A:1075:ARG:HG2	1:A:1086:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ALA:H	1:A:1437:LEU:HD21	1.74	0.53
1:B:205:SER:HB2	1:B:379:ALA:HB1	1.89	0.53
1:A:12:TYR:HE1	3:I:70:TYR:HB2	1.73	0.53
1:A:255:LYS:HB2	1:A:261:ALA:HA	1.91	0.53
1:B:631:GLY:HA3	1:B:636:GLU:HA	1.89	0.53
1:A:1181:VAL:HG13	1:A:1200:PRO:HA	1.91	0.53
1:B:1077:THR:HG22	1:B:1083:PRO:HA	1.90	0.53
1:B:112:SER:HB3	1:B:115:GLU:HG2	1.90	0.53
1:A:291:VAL:HG23	1:A:453:GLU:HB3	1.91	0.52
1:A:329:PRO:HB3	1:A:357:TYR:HD1	1.73	0.52
1:B:22:ALA:O	1:B:25:GLN:HG3	2.09	0.52
1:B:1123:PHE:HB3	1:B:1195:VAL:HG21	1.91	0.52
1:B:672:MET:HE1	1:B:733:SER:H	1.74	0.52
1:B:1135:LEU:HD21	1:B:1325:LEU:HB3	1.92	0.52
1:A:738:VAL:HB	1:A:786:ARG:HD2	1.91	0.52
1:A:829:THR:HG22	1:A:830:LEU:HG	1.92	0.52
1:A:1049:PRO:HA	1:A:1092:GLY:HA2	1.91	0.52
2:K:39:VAL:HG12	2:K:99:TYR:HB2	1.90	0.52
3:I:104:VAL:HA	3:I:126:VAL:HG13	1.90	0.52
1:B:232:VAL:HA	1:B:268:GLU:HG2	1.91	0.52
1:B:1232:VAL:HG22	1:B:1309:ALA:HB3	1.90	0.52
2:J:162:ASN:HB2	2:J:165:ALA:HB3	1.92	0.52
1:A:1403:TRP:HA	1:A:1429:LEU:HB2	1.92	0.52
1:B:515:ARG:HB2	1:B:849:VAL:HG23	1.92	0.52
2:J:204:ASN:HB2	2:J:213:LYS:HZ1	1.75	0.52
3:I:130:ARG:HD2	3:I:193:SER:HB2	1.92	0.52
1:B:831:ARG:HB3	1:B:834:ASP:HB3	1.92	0.52
3:I:215:ALA:HA	3:I:229:LYS:O	2.09	0.52
1:A:555:TRP:CD1	1:A:832:ARG:HG2	2.45	0.52
1:A:589:VAL:HG22	1:A:593:ARG:HE	1.75	0.52
1:A:1424:ILE:HD12	1:A:1472:LEU:HD11	1.92	0.52
1:B:292:LEU:HD22	1:B:450:LEU:HD12	1.92	0.52
1:A:112:SER:HB2	1:A:1517:LEU:HB3	1.92	0.52
3:L:97:SER:C	3:L:98:ARG:HG2	2.34	0.52
1:A:1527:SER:HA	1:A:1567:PRO:HG2	1.92	0.51
1:B:546:TRP:CD2	1:B:626:PRO:HB3	2.45	0.51
1:B:1552:THR:HG23	1:B:1554:LEU:H	1.75	0.51
1:A:427:TRP:CZ2	1:A:434:ARG:HB3	2.45	0.51
1:B:361:ARG:HH12	1:B:365:LEU:HG	1.73	0.51
1:B:1472:LEU:HD22	1:B:1475:LEU:HD12	1.91	0.51
1:A:814:VAL:HG23	1:A:815:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:GLU:HA	1:A:977:ARG:HH21	1.75	0.51
3:I:52:ASN:O	3:I:71:LEU:HD13	2.10	0.51
1:A:580:LEU:HD13	1:A:652:ALA:HB1	1.91	0.51
1:A:1067:VAL:HG22	1:A:1076:LEU:HD22	1.91	0.51
3:L:147:LEU:HB3	3:L:205:LYS:HE2	1.93	0.51
1:B:134:LEU:HD21	1:B:144:LEU:HD12	1.92	0.51
1:B:1403:TRP:HZ3	1:B:1434:GLY:HA3	1.75	0.51
3:I:185:VAL:HG22	3:I:197:LEU:HD13	1.91	0.51
1:A:945:VAL:HA	1:A:998:LEU:HD12	1.91	0.51
1:B:1421:ASN:HB3	1:B:1426:MET:HB3	1.92	0.51
1:B:26:ARG:O	1:B:29:GLU:HG3	2.10	0.51
1:B:662:ILE:HD11	1:B:731:TYR:CD2	2.46	0.51
1:B:904:ARG:HH21	1:B:967:ILE:HD13	1.76	0.51
1:A:912:SER:HB2	1:A:914:ARG:HH21	1.75	0.51
1:A:1164:ALA:HB1	1:A:1376:ALA:HB1	1.93	0.51
3:L:171:LYS:O	3:L:215:ALA:HB3	2.10	0.51
1:B:926:ASN:HA	1:B:929:LEU:HD23	1.92	0.50
1:B:1233:LEU:HG	1:B:1259:VAL:HB	1.92	0.50
1:A:1108:VAL:HG21	1:A:1365:VAL:HG21	1.93	0.50
1:B:24:ARG:O	1:B:27:ILE:HG23	2.12	0.50
1:B:491:LEU:HD13	1:B:869:PRO:HD3	1.94	0.50
2:J:68:VAL:HB	2:J:72:PHE:HD2	1.76	0.50
1:A:4:THR:HB	1:A:8:LYS:HE2	1.94	0.50
1:B:1511:ARG:HH12	1:B:1512:HIS:CE1	2.29	0.50
1:B:164:ALA:HB3	1:B:883:ALA:H	1.77	0.50
1:A:441:PHE:HD1	1:A:447:ASN:HB3	1.76	0.50
1:B:912:SER:HB3	1:B:961:SER:HB3	1.94	0.50
1:A:985:GLU:H	1:A:988:GLU:HG2	1.77	0.50
1:A:1322:VAL:HG22	1:A:1372:ALA:HB2	1.94	0.50
1:B:156:MET:HE3	1:B:156:MET:HA	1.92	0.50
1:B:398:LEU:HG	1:B:427:TRP:HB2	1.93	0.50
1:A:903:ASP:HB3	1:A:970:GLU:HG2	1.93	0.50
1:B:121:PRO:O	1:B:125:LEU:HD22	2.12	0.50
1:B:353:LEU:HA	1:B:356:THR:HG22	1.93	0.50
1:B:544:VAL:HA	1:B:805:VAL:HB	1.93	0.50
3:I:119:THR:HG23	3:I:121:GLY:H	1.77	0.50
1:A:654:VAL:HG22	1:A:749:LEU:HD22	1.94	0.50
1:B:1237:GLY:HA2	1:B:1242:GLY:HA3	1.94	0.50
2:K:14:VAL:HG21	2:K:20:LEU:HD22	1.94	0.50
2:K:72:PHE:HB3	2:K:85:LEU:HD11	1.94	0.50
1:A:13:LEU:O	1:A:17:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:VAL:HA	1:A:686:LEU:HD12	1.94	0.50
1:A:1538:4HH:HT2	1:B:443:VAL:HB	1.93	0.50
1:B:1111:PRO:HD2	1:B:1211:VAL:O	2.12	0.50
1:B:1261:VAL:HB	1:B:1286:CYS:HB3	1.92	0.50
2:K:62:THR:HB	2:K:74:ILE:HD11	1.93	0.50
2:J:64:TYR:CE2	2:J:74:ILE:HG12	2.46	0.49
1:A:1483:ALA:HB2	1:B:1059:ALA:HB1	1.94	0.49
1:B:904:ARG:HA	1:B:968:VAL:O	2.12	0.49
1:B:908:VAL:HG22	1:B:965:GLN:HG2	1.94	0.49
1:B:942:THR:HA	1:B:1000:PRO:HA	1.93	0.49
1:A:1232:VAL:HB	1:A:1258:LEU:HD23	1.94	0.49
1:A:1311:ILE:HG23	1:A:1357:VAL:HB	1.93	0.49
1:B:204:SER:HB3	1:B:440:SER:HB3	1.93	0.49
3:L:60:LYS:HB2	3:L:63:GLN:HB3	1.94	0.49
1:B:336:GLU:HG3	1:B:389:MET:SD	2.53	0.49
1:B:370:LEU:HD12	1:B:385:GLY:HA2	1.95	0.49
1:B:776:LEU:HD12	1:B:781:TRP:CH2	2.48	0.49
1:B:910:GLN:HE22	1:B:963:GLU:HB2	1.77	0.49
3:I:30:THR:HG23	3:I:129:LYS:HB3	1.95	0.49
1:A:516:ALA:HB1	1:A:533:LEU:HD21	1.95	0.49
1:B:670:GLY:CA	1:B:705:GLY:O	2.61	0.49
1:B:685:ARG:NH2	1:B:716:ILE:HB	2.21	0.49
3:I:47:HIS:HB3	3:I:49:ASN:OD1	2.13	0.49
1:B:104:PHE:CD1	1:B:124:ARG:HB3	2.48	0.49
3:I:144:ASP:HA	3:I:147:LEU:HD12	1.95	0.49
1:B:765:VAL:HA	1:B:790:ARG:HH22	1.78	0.49
1:B:1105:LEU:HD13	1:B:1448:LEU:HD13	1.94	0.49
1:B:1204:VAL:HG22	1:B:1209:ALA:HB2	1.95	0.49
2:K:74:ILE:HG23	2:K:85:LEU:HD13	1.95	0.49
3:L:19:VAL:HG13	3:L:42:SER:OG	2.12	0.49
3:L:118:LEU:HD23	3:L:119:THR:H	1.78	0.49
1:A:12:TYR:CZ	3:I:71:LEU:HD23	2.48	0.48
1:A:45:PRO:HD3	1:A:98:LEU:HG	1.95	0.48
1:A:174:THR:HG21	1:B:241:GLU:HG2	1.96	0.48
2:K:40:ARG:HH22	2:K:94:ASP:HA	1.77	0.48
3:I:167:LYS:NZ	3:I:169:GLN:HB2	2.29	0.48
1:A:15:ARG:HD3	2:J:108:ASP:HB2	1.95	0.48
1:A:292:LEU:HD23	1:A:450:LEU:HD11	1.95	0.48
1:A:764:THR:HG21	1:A:789:VAL:HG13	1.94	0.48
1:A:1321:VAL:HA	1:A:1370:GLY:HA2	1.94	0.48
1:A:205:SER:HB2	1:A:379:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:HA	1:A:805:VAL:HG23	1.94	0.48
1:A:622:VAL:HG23	1:A:624:VAL:HG23	1.95	0.48
1:A:1400:TRP:H	1:A:1400:TRP:CD1	2.29	0.48
1:B:811:ALA:HA	1:B:830:LEU:HB2	1.95	0.48
1:B:841:LEU:HD22	1:B:844:MET:HE3	1.94	0.48
1:A:60:GLU:HG3	1:A:62:VAL:HG23	1.94	0.48
1:A:1134:THR:HG21	1:A:1165:ILE:HG23	1.96	0.48
1:B:1233:LEU:HD11	1:B:1297:VAL:HG12	1.96	0.48
1:A:820:SER:HA	1:A:824:GLY:H	1.78	0.48
1:A:1429:LEU:HD11	1:A:1451:ALA:HA	1.95	0.48
3:L:19:VAL:HG13	3:L:42:SER:H	1.78	0.48
1:A:509:ARG:NH2	1:A:868:LEU:HB2	2.29	0.48
2:K:213:LYS:HD2	2:K:213:LYS:HA	1.64	0.48
3:I:68:LEU:HA	3:I:79:VAL:HG21	1.95	0.48
1:B:255:LYS:HB3	1:B:258:ALA:HB3	1.95	0.48
1:B:546:TRP:CG	1:B:626:PRO:HB3	2.48	0.48
1:B:1469:PRO:HD2	1:B:1472:LEU:HB2	1.95	0.48
3:I:98:ARG:NE	3:I:98:ARG:HA	2.29	0.48
1:A:224:MET:HB3	1:A:224:MET:HE2	1.80	0.48
1:A:546:TRP:CE2	1:A:626:PRO:HB3	2.49	0.48
1:B:72:ARG:HD2	1:B:879:TRP:CZ2	2.48	0.48
1:A:776:LEU:HD12	1:A:781:TRP:HH2	1.78	0.48
1:A:984:ARG:HB2	1:A:988:GLU:HG3	1.95	0.48
1:A:381:ALA:O	1:A:384:ALA:HB3	2.14	0.47
1:A:1342:ARG:HE	1:A:1384:LEU:HD21	1.80	0.47
1:A:1556:LEU:HD12	1:A:1560:MET:HE2	1.95	0.47
1:B:82:PRO:HA	1:B:84:ARG:HH22	1.79	0.47
2:K:72:PHE:CE1	2:K:87:MET:HB2	2.49	0.47
3:I:153:SER:HA	3:I:201:LEU:O	2.14	0.47
1:B:622:VAL:HG23	1:B:624:VAL:HG23	1.95	0.47
1:B:1516:VAL:HG23	1:B:1547:ARG:HH21	1.80	0.47
1:A:76:LEU:HD23	1:A:76:LEU:H	1.79	0.47
1:A:754:ALA:HB3	1:A:774:GLY:HA2	1.95	0.47
1:B:778:GLY:HA2	1:B:781:TRP:HD1	1.79	0.47
2:J:36:MET:HE2	2:J:36:MET:N	2.28	0.47
3:L:162:TYR:HB2	3:L:194:THR:HG22	1.94	0.47
1:A:928:ALA:HB2	1:A:1032:PRO:HB3	1.97	0.47
1:B:1134:THR:HG21	1:B:1165:ILE:HG23	1.97	0.47
1:B:1288:VAL:HA	1:B:1294:LEU:HD13	1.96	0.47
2:J:105:THR:HG23	3:I:117:ARG:HH22	1.80	0.47
1:A:1008:PRO:HB2	1:A:1070:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1248:HIS:CD2	1:B:1435:MET:HB3	2.50	0.47
2:J:72:PHE:CD1	2:J:87:MET:HA	2.50	0.47
2:J:80:LYS:HB2	2:J:82:ILE:HG22	1.96	0.47
2:K:144:ALA:HB2	2:K:190:THR:HG22	1.95	0.47
1:A:1232:VAL:HG22	1:A:1309:ALA:HB3	1.97	0.47
1:B:86:ARG:HD3	1:B:89:THR:HG21	1.97	0.47
1:B:670:GLY:HA3	1:B:705:GLY:O	2.14	0.47
1:B:1118:ALA:HB3	1:B:1193:ALA:HA	1.96	0.47
2:J:4:VAL:HG22	2:J:29:PHE:HB3	1.97	0.47
2:J:72:PHE:HA	2:J:86:GLN:O	2.14	0.47
3:I:140:PHE:HB2	3:I:155:VAL:HG23	1.96	0.47
1:A:685:ARG:HH22	1:A:716:ILE:HG13	1.79	0.47
1:B:276:GLU:HG3	1:B:281:ALA:HB2	1.97	0.47
1:B:580:LEU:HD11	1:B:652:ALA:HB1	1.96	0.47
1:B:671:GLY:C	1:B:672:MET:HE2	2.39	0.47
1:A:666:LEU:O	1:A:731:TYR:HB3	2.15	0.47
1:B:1437:LEU:HD13	1:B:1450:ALA:HB1	1.97	0.47
1:B:1505:LEU:HD23	1:B:1508:LEU:HD21	1.97	0.47
1:A:673:ALA:HB3	1:A:703:ILE:HD11	1.96	0.47
1:B:158:GLN:HG3	1:B:232:VAL:O	2.15	0.47
1:B:1325:LEU:HD12	1:B:1372:ALA:HB3	1.96	0.47
2:J:35:ALA:C	2:J:36:MET:HE2	2.40	0.47
2:J:154:PRO:HA	2:J:183:TYR:HE2	1.79	0.47
1:A:1325:LEU:HD13	1:A:1330:LEU:HD21	1.98	0.46
1:A:244:ARG:HH12	1:B:171:GLY:HA3	1.80	0.46
1:B:672:MET:HE2	1:B:672:MET:N	2.30	0.46
1:B:1110:TRP:HA	1:B:1211:VAL:O	2.15	0.46
1:B:1286:CYS:HA	1:B:1293:GLN:HG2	1.97	0.46
2:K:161:TRP:HB3	2:K:166:LEU:HB3	1.97	0.46
1:A:117:VAL:HG12	1:A:878:TYR:HB3	1.98	0.46
1:B:675:VAL:HA	1:B:724:VAL:HG12	1.97	0.46
1:B:1399:ALA:O	1:B:1449:VAL:HG13	2.16	0.46
3:L:20:MET:SD	3:L:20:MET:N	2.88	0.46
1:A:55:TRP:HH2	1:A:397:THR:HB	1.80	0.46
1:A:125:LEU:HD11	1:A:270:VAL:HG21	1.97	0.46
1:B:658:ARG:NH2	1:B:745:LEU:HD13	2.30	0.46
1:A:383:VAL:O	1:A:387:ILE:HG12	2.15	0.46
1:B:14:ARG:HB3	3:I:51:TYR:OH	2.15	0.46
2:K:14:VAL:O	2:K:118:VAL:HA	2.14	0.46
3:L:218:VAL:O	3:L:226:PRO:HA	2.16	0.46
1:B:1070:THR:HG23	1:B:1074:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1358:LEU:HD12	1:B:1385:ALA:HB2	1.98	0.46
2:J:16:PRO:HG3	2:J:118:VAL:HG12	1.98	0.46
2:K:155:GLU:HG2	2:K:183:TYR:CE2	2.51	0.46
2:J:54:ARG:HH11	2:J:61:THR:HG23	1.81	0.46
1:A:653:LYS:O	1:A:657:LEU:HG	2.16	0.46
1:A:1399:ALA:HB3	1:A:1449:VAL:HA	1.97	0.46
1:A:1531:PHE:HD2	1:A:1561:ILE:HG13	1.80	0.46
2:K:98:TYR:C	2:K:99:TYR:HD1	2.24	0.46
3:L:160:ASN:HA	3:L:194:THR:OG1	2.16	0.46
3:L:191:LYS:HA	3:L:191:LYS:HE3	1.98	0.46
1:A:94:GLN:HE22	1:A:253:ARG:HH22	1.63	0.46
1:B:1455:VAL:O	1:B:1459:ARG:HG2	2.14	0.46
1:A:976:ARG:HA	1:A:998:LEU:O	2.16	0.45
1:A:1110:TRP:CZ3	1:A:1212:PRO:HD3	2.52	0.45
1:B:1040:ARG:HH11	1:B:1045:ASP:HA	1.81	0.45
1:B:1338:VAL:HG21	1:B:1380:GLU:HB3	1.98	0.45
2:K:14:VAL:HG11	2:K:90:LEU:HD12	1.97	0.45
1:A:566:SER:OG	1:A:569:PHE:HB3	2.16	0.45
1:A:364:PRO:HA	1:A:417:ALA:HB1	1.99	0.45
1:A:846:GLU:O	1:A:850:ARG:HG2	2.15	0.45
1:A:1115:LEU:HD23	1:A:1115:LEU:HA	1.82	0.45
3:L:215:ALA:HA	3:L:230:SER:HA	1.98	0.45
1:B:24:ARG:HH21	3:I:75:ARG:CZ	2.30	0.45
1:B:555:TRP:CG	1:B:832:ARG:HG3	2.51	0.45
2:J:166:LEU:HD21	2:J:189:VAL:HG11	1.98	0.45
2:K:90:LEU:HB3	2:K:118:VAL:HG21	1.99	0.45
1:A:489:ALA:O	1:A:493:GLU:HG2	2.15	0.45
1:A:583:TRP:CZ2	1:A:653:LYS:HE3	2.51	0.45
1:A:1380:GLU:O	1:A:1384:LEU:HG	2.16	0.45
3:I:29:VAL:HG21	3:I:35:ALA:HB2	1.98	0.45
1:A:1076:LEU:HD12	1:A:1085:LEU:HD23	1.98	0.45
1:B:566:SER:OG	1:B:569:PHE:HB3	2.17	0.45
1:B:1315:GLY:HA3	1:B:1337:LYS:HE2	1.97	0.45
1:A:312:LEU:HB3	1:A:316:ARG:HH22	1.82	0.45
1:A:1338:VAL:HG13	1:A:1384:LEU:HD11	1.99	0.45
1:B:1403:TRP:CD2	1:B:1409:MET:HE3	2.52	0.45
2:K:204:ASN:HB3	2:K:213:LYS:HZ1	1.81	0.45
3:L:188:GLN:HB2	3:L:195:TYR:CE1	2.52	0.45
1:A:248:LEU:HA	1:A:264:THR:H	1.82	0.45
1:A:348:ILE:O	1:A:351:GLN:HG2	2.17	0.45
1:A:900:PRO:HA	1:B:990:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:135:PRO:HB3	3:I:161:PHE:HB3	1.99	0.45
1:A:723:ARG:NH1	1:A:725:ARG:HB2	2.31	0.44
1:A:1410:THR:HG22	1:A:1413:LEU:HD12	1.99	0.44
1:B:377:ALA:H	1:B:381:ALA:HB2	1.82	0.44
1:B:958:ARG:HG3	1:B:959:ARG:HD2	1.98	0.44
1:B:1526:HIS:H	1:B:1529:ARG:NH2	2.15	0.44
1:A:815:THR:C	1:A:818:PRO:HD2	2.42	0.44
1:A:911:TRP:CD2	1:A:964:VAL:HG21	2.53	0.44
1:A:1399:ALA:HB3	1:A:1449:VAL:HG22	1.98	0.44
1:B:365:LEU:HB2	1:B:418:ILE:HG13	2.00	0.44
1:B:1049:PRO:HA	1:B:1092:GLY:HA2	2.00	0.44
1:A:24:ARG:HA	1:A:27:ILE:HG23	1.99	0.44
1:A:27:ILE:HB	1:B:27:ILE:HB	1.99	0.44
1:B:659:SER:HA	1:B:662:ILE:HG22	1.99	0.44
3:I:75:ARG:CZ	3:I:81:ASP:HA	2.48	0.44
1:A:1111:PRO:HD2	1:A:1211:VAL:O	2.16	0.44
1:B:1473:ARG:CZ	1:B:1478:LEU:H	2.31	0.44
1:B:1488:SER:HB3	1:B:1491:GLU:CD	2.42	0.44
1:B:589:VAL:HG22	1:B:593:ARG:HE	1.83	0.44
2:K:64:TYR:CE2	2:K:74:ILE:HG13	2.53	0.44
3:I:31:PRO:HA	3:I:99:VAL:HB	1.99	0.44
1:A:151:VAL:HG12	1:A:226:LEU:HB2	2.00	0.44
1:A:615:LEU:HD13	1:A:829:THR:HG21	1.99	0.44
1:A:1077:THR:HG22	1:A:1083:PRO:HA	1.99	0.44
1:A:1102:THR:OG1	1:A:1219:PRO:HG2	2.18	0.44
1:A:1548:LEU:HD11	1:A:1574:LEU:HD11	2.00	0.44
1:B:1345:ASP:HB2	1:B:1388:ARG:HD2	2.00	0.44
1:B:1538:4HH:HP2	1:B:1538:4HH:HS2	1.63	0.44
1:A:124:ARG:HH12	1:A:878:TYR:HB2	1.82	0.44
1:A:1426:MET:HG3	1:A:1453:PHE:CE1	2.53	0.44
1:B:1310:VAL:HG11	1:B:1344:LEU:HD22	1.98	0.44
3:I:29:VAL:O	3:I:128:ILE:HD12	2.18	0.44
1:A:245:GLN:HE21	1:B:1539:LEU:HD21	1.82	0.44
1:A:1505:LEU:HD12	1:A:1505:LEU:H	1.83	0.44
1:A:1527:SER:HB3	1:A:1568:PRO:HD3	2.00	0.44
1:B:330:SER:HA	1:B:361:ARG:HD3	1.99	0.44
1:B:1334:ARG:HG2	1:B:1338:VAL:HB	2.00	0.44
2:K:128:VAL:HG21	2:K:214:VAL:HG11	1.98	0.44
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.87	0.44
1:A:546:TRP:CD2	1:A:626:PRO:HB3	2.53	0.44
1:A:1219:PRO:HB3	1:A:1440:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ARG:HH21	1:B:868:LEU:HB3	1.82	0.44
3:L:102:GLU:OE2	3:L:102:GLU:N	2.50	0.44
1:A:768:GLU:HG2	1:A:769:TRP:N	2.33	0.43
1:A:1107:ARG:HD2	1:A:1108:VAL:H	1.83	0.43
1:A:1473:ARG:HH21	1:A:1478:LEU:N	2.15	0.43
1:B:729:VAL:HG13	1:B:731:TYR:CE1	2.53	0.43
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.86	0.43
1:A:1135:LEU:HB2	1:A:1168:LEU:HD11	1.99	0.43
1:B:427:TRP:CZ2	1:B:434:ARG:HB3	2.53	0.43
2:J:85:LEU:HD12	2:J:86:GLN:H	1.82	0.43
1:A:211:HIS:HD2	1:A:212:LEU:HD22	1.82	0.43
1:A:1401:GLY:HA3	1:A:1426:MET:HE1	2.00	0.43
1:B:1353:LEU:HD12	1:B:1388:ARG:HH22	1.83	0.43
2:J:4:VAL:HA	2:J:27:SER:O	2.18	0.43
1:A:407:PRO:HB2	1:A:413:TRP:NE1	2.33	0.43
1:A:1029:GLY:O	1:A:1030:ILE:HD13	2.18	0.43
3:L:170:TRP:CG	3:L:201:LEU:HD13	2.52	0.43
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.74	0.43
1:A:351:GLN:HA	1:A:354:LEU:HB2	2.01	0.43
1:A:364:PRO:HB2	1:A:419:GLU:OE1	2.19	0.43
1:A:601:VAL:HG11	1:A:731:TYR:CE1	2.50	0.43
1:A:788:GLN:HB2	1:A:790:ARG:CZ	2.49	0.43
1:B:591:VAL:HG12	1:B:596:GLY:HA3	1.99	0.43
1:B:796:THR:HA	1:B:799:LEU:HD12	2.00	0.43
1:B:1473:ARG:NE	1:B:1478:LEU:H	2.17	0.43
3:L:111:GLN:HE22	3:L:114:GLN:HB3	1.83	0.43
1:A:819:LEU:HD11	1:A:826:ALA:HB2	2.00	0.43
1:A:942:THR:HA	1:A:1000:PRO:HA	2.00	0.43
3:L:70:TYR:HE2	3:L:76:ALA:HB2	1.83	0.43
1:A:565:GLU:OE1	1:A:837:LEU:HB2	2.18	0.43
1:A:831:ARG:HB3	1:A:834:ASP:HB3	2.01	0.43
1:A:1105:LEU:HB3	1:A:1448:LEU:HB3	2.00	0.43
1:B:305:GLY:H	1:B:308:ALA:HB3	1.83	0.43
1:B:623:GLY:HA2	1:B:625:ARG:HH12	1.82	0.43
1:B:1357:VAL:HA	1:B:1396:VAL:O	2.18	0.43
2:J:213:LYS:HA	2:J:213:LYS:HD2	1.85	0.43
3:I:107:TYR:HE1	3:I:126:VAL:HG11	1.84	0.43
3:I:147:LEU:HB3	3:I:205:LYS:HD3	2.01	0.43
1:A:645:ALA:HB2	1:A:757:PRO:HB3	2.00	0.43
1:B:1526:HIS:CE1	1:B:1529:ARG:HE	2.36	0.43
1:B:1531:PHE:HD2	1:B:1561:ILE:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:SER:HA	2:J:87:MET:O	2.18	0.43
2:K:20:LEU:HB3	2:K:87:MET:SD	2.59	0.43
1:A:311:GLY:O	1:A:315:GLN:HG2	2.19	0.43
1:A:491:LEU:HD22	1:A:869:PRO:HD3	2.01	0.43
1:B:858:ALA:HB3	1:B:859:MET:HE3	2.00	0.43
1:B:1311:ILE:HG23	1:B:1357:VAL:HB	2.00	0.43
2:J:201:TYR:H	2:J:217:LYS:NZ	2.15	0.43
3:L:145:GLU:CD	3:L:145:GLU:H	2.26	0.43
1:A:1:MET:HE1	3:I:18:VAL:HA	2.01	0.43
2:J:68:VAL:HB	2:J:72:PHE:CD2	2.52	0.43
1:A:171:GLY:HA3	1:B:244:ARG:NH2	2.25	0.42
1:A:657:LEU:HA	1:A:660:GLN:OE1	2.18	0.42
1:B:13:LEU:O	1:B:17:THR:HG23	2.19	0.42
1:A:998:LEU:HD12	1:A:998:LEU:HA	1.89	0.42
1:B:1359:PHE:CE1	1:B:1398:ILE:HD11	2.54	0.42
3:L:168:VAL:HA	3:L:217:GLU:O	2.20	0.42
1:A:580:LEU:HD11	1:A:656:ALA:HB2	2.01	0.42
1:A:778:GLY:HA2	1:A:781:TRP:CD1	2.53	0.42
1:B:314:GLN:HA	1:B:317:VAL:HG12	2.01	0.42
1:B:1566:LYS:HD3	1:B:1566:LYS:HA	1.70	0.42
3:I:128:ILE:HG22	3:I:188:GLN:CD	2.44	0.42
2:K:101:THR:HG21	2:K:107:PHE:HB3	2.01	0.42
3:I:95:LYS:NZ	3:I:97:SER:HB3	2.34	0.42
1:A:152:PHE:O	1:A:227:ALA:HA	2.19	0.42
1:A:918:TRP:HB2	1:A:1033:ALA:HB2	2.01	0.42
1:A:231:THR:HG21	1:A:379:ALA:H	1.84	0.42
1:A:411:VAL:HB	1:A:413:TRP:CE2	2.55	0.42
1:A:1538:4HH:HL3	1:A:1538:4HH:HO3	1.70	0.42
1:B:54:LEU:O	1:B:58:VAL:HG23	2.19	0.42
1:B:576:CYS:O	1:B:580:LEU:HD23	2.20	0.42
1:B:1294:LEU:HD23	1:B:1347:LEU:HD12	2.01	0.42
1:B:1313:THR:HG22	1:B:1359:PHE:CD1	2.54	0.42
1:B:1361:SER:HB3	1:B:1378:ASN:ND2	2.35	0.42
1:A:72:ARG:HD2	1:A:879:TRP:CZ2	2.54	0.42
1:A:433:PRO:HB2	1:A:435:ARG:CZ	2.49	0.42
1:B:239:PHE:HE1	1:B:266:TRP:HB2	1.84	0.42
1:A:35:ILE:HD12	1:A:277:ARG:HA	2.02	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.92	0.42
1:A:472:VAL:HG12	1:A:517:VAL:HG22	2.02	0.42
1:A:1313:THR:HA	1:A:1359:PHE:HB2	2.02	0.42
2:K:149:VAL:HG23	2:K:152:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASP:OD1	1:A:310:ASN:HB3	2.19	0.42
1:A:1366:LEU:HD13	1:A:1471:LEU:HB3	2.01	0.42
1:A:1504:ALA:HA	1:A:1507:ASP:OD2	2.20	0.42
3:I:58:LEU:HG	3:I:60:LYS:NZ	2.35	0.42
3:L:119:THR:HG23	3:L:121:GLY:H	1.84	0.42
1:A:398:LEU:HG	1:A:427:TRP:HB2	2.02	0.42
1:B:1211:VAL:HB	1:B:1213:ARG:NH1	2.35	0.42
1:A:264:THR:HG22	1:A:340:THR:O	2.20	0.41
1:B:1067:VAL:HG22	1:B:1076:LEU:HD22	2.01	0.41
1:B:1463:LYS:HA	1:B:1463:LYS:HD2	1.79	0.41
2:K:31:PHE:CD2	2:K:81:SER:HA	2.55	0.41
2:K:146:GLY:HA2	2:K:161:TRP:CZ2	2.55	0.41
3:L:58:LEU:HG	3:L:66:GLN:HB3	2.01	0.41
1:A:8:LYS:O	1:A:11:GLU:HG3	2.19	0.41
1:A:289:LEU:HA	1:A:394:ARG:HH22	1.85	0.41
1:A:329:PRO:HB3	1:A:357:TYR:CD1	2.54	0.41
1:A:1248:HIS:CD2	1:A:1435:MET:HB3	2.55	0.41
1:B:61:ARG:NH2	1:B:423:GLU:HA	2.35	0.41
1:B:1110:TRP:HB3	1:B:1210:SER:HB2	2.02	0.41
2:K:97:VAL:HA	2:K:115:LEU:HA	2.02	0.41
1:A:183:SER:HA	1:A:186:VAL:HG12	2.01	0.41
1:A:327:LEU:HD11	1:A:435:ARG:NE	2.35	0.41
1:A:1538:4HH:HR	1:A:1538:4HH:HO2	1.40	0.41
1:B:813:PRO:HD3	1:B:830:LEU:O	2.20	0.41
1:B:1104:ALA:H	1:B:1437:LEU:HD21	1.85	0.41
1:B:1345:ASP:CB	1:B:1388:ARG:HD2	2.50	0.41
1:B:1538:4HH:HL3	1:B:1538:4HH:HO3	1.71	0.41
2:J:8:GLN:H	2:J:112:GLN:NE2	2.18	0.41
3:I:127:ASP:HB2	3:I:188:GLN:OE1	2.19	0.41
1:A:1168:LEU:HG	1:A:1372:ALA:HB1	2.02	0.41
1:B:1249:LEU:HD13	1:B:1255:VAL:HG21	2.03	0.41
1:B:1429:LEU:HD21	1:B:1452:LYS:H	1.86	0.41
2:J:145:LEU:HB2	2:J:218:VAL:HG11	2.03	0.41
1:A:125:LEU:HD21	1:A:270:VAL:HG22	2.01	0.41
1:A:178:ALA:HB3	1:A:181:VAL:HG23	2.01	0.41
1:A:479:GLU:HG2	1:A:480:SER:N	2.36	0.41
1:A:670:GLY:HA3	1:A:732:ALA:HB2	2.02	0.41
1:A:1361:SER:HA	1:A:1400:TRP:O	2.20	0.41
1:B:473:VAL:HG22	1:B:516:ALA:HB3	2.03	0.41
1:B:565:GLU:OE1	1:B:837:LEU:HB2	2.20	0.41
1:B:1473:ARG:HE	1:B:1477:PRO:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:129:PHE:HB3	3:I:143:SER:HB3	2.02	0.41
2:K:29:PHE:CE2	2:K:31:PHE:HA	2.55	0.41
1:A:108:PHE:HA	1:A:476:ARG:HD2	2.01	0.41
1:A:474:SER:HA	1:A:514:GLU:O	2.21	0.41
1:A:631:GLY:HA3	1:A:636:GLU:HA	2.02	0.41
1:A:813:PRO:HD3	1:A:830:LEU:O	2.21	0.41
1:B:183:SER:HA	1:B:186:VAL:HG12	2.01	0.41
1:A:665:GLU:HG3	1:A:741:ILE:HG21	2.03	0.41
1:A:1112:GLU:HA	1:A:1209:ALA:O	2.20	0.41
1:B:276:GLU:OE2	1:B:280:VAL:HB	2.20	0.41
1:B:1526:HIS:H	1:B:1529:ARG:HH21	1.67	0.41
2:J:19:SER:HB3	2:J:86:GLN:HE21	1.85	0.41
3:L:54:LEU:HD22	3:L:92:PHE:CG	2.56	0.41
1:B:12:TYR:CE1	2:K:106:LEU:HD21	2.54	0.41
1:B:1490:THR:HA	1:B:1493:LEU:HD12	2.02	0.41
2:J:48:GLU:OE1	2:J:48:GLU:N	2.54	0.41
1:A:76:LEU:O	1:A:80:ILE:HG12	2.21	0.41
1:A:586:TRP:HE1	1:A:591:VAL:HG21	1.85	0.41
1:A:812:HIS:CG	1:A:832:ARG:HG3	2.55	0.41
1:A:837:LEU:HG	1:A:841:LEU:HD23	2.02	0.41
1:A:892:LEU:HA	1:A:911:TRP:NE1	2.36	0.41
1:A:893:LEU:HD11	1:A:935:ARG:HB3	2.01	0.41
1:A:1182:LEU:HB2	1:A:1200:PRO:O	2.21	0.41
1:A:1235:THR:HB	1:A:1288:VAL:HG11	2.02	0.41
1:A:1358:LEU:HD13	1:A:1381:LEU:HG	2.03	0.41
1:A:1403:TRP:CZ3	1:A:1431:ALA:HA	2.55	0.41
1:A:1510:ARG:HH21	1:A:1523:GLU:HA	1.85	0.41
1:B:742:ARG:HG2	1:B:782:TYR:CE1	2.56	0.41
1:B:850:ARG:HD3	1:B:850:ARG:HA	1.82	0.41
2:J:31:PHE:HZ	2:J:76:ARG:HB2	1.85	0.41
2:J:47:LEU:HD11	3:I:120:PHE:CG	2.56	0.41
2:J:202:ILE:HG23	2:J:215:ASP:OD1	2.21	0.41
2:K:80:LYS:HB2	2:K:82:ILE:HG12	2.02	0.41
3:I:170:TRP:CD1	3:I:201:LEU:HD13	2.55	0.41
3:L:54:LEU:HD22	3:L:92:PHE:CD2	2.55	0.41
3:L:108:TYR:CD2	3:L:120:PHE:HB3	2.56	0.41
1:A:35:ILE:HD12	1:A:35:ILE:HA	1.89	0.41
1:A:488:LEU:HD13	1:A:488:LEU:HA	1.92	0.41
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.91	0.41
1:A:685:ARG:HH12	1:A:716:ILE:HD12	1.86	0.41
1:A:846:GLU:HA	1:A:849:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:SER:HB2	1:A:914:ARG:HE	1.86	0.41
1:A:1561:ILE:HG23	1:A:1562:PHE:HD1	1.85	0.41
1:B:512:LEU:HD13	1:B:512:LEU:HA	1.91	0.41
1:A:344:LEU:O	1:A:347:PRO:HD2	2.21	0.40
1:A:572:ARG:HA	1:A:572:ARG:HD2	1.80	0.40
1:A:1057:LEU:HD12	1:A:1085:LEU:HB2	2.03	0.40
1:A:1287:ASP:HB3	1:A:1290:ASP:HB2	2.02	0.40
1:A:1569:ALA:HA	1:A:1572:ASP:OD2	2.21	0.40
1:B:549:PRO:HG3	1:B:808:GLU:HG3	2.03	0.40
1:B:636:GLU:O	1:B:639:ALA:HB3	2.21	0.40
1:B:890:ASP:HB3	1:B:893:LEU:HB2	2.03	0.40
3:L:118:LEU:HD23	3:L:119:THR:N	2.35	0.40
1:A:937:GLY:HA2	1:A:940:ALA:HB3	2.03	0.40
1:A:1217:VAL:HG21	1:A:1448:LEU:HD22	2.02	0.40
1:A:1325:LEU:HD23	1:A:1325:LEU:HA	1.88	0.40
1:B:84:ARG:HB3	1:B:246:ARG:HH21	1.86	0.40
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.86	0.40
1:B:799:LEU:HD21	1:B:823:THR:HB	2.02	0.40
1:B:1325:LEU:HD23	1:B:1325:LEU:HA	1.92	0.40
2:J:19:SER:HB3	2:J:86:GLN:NE2	2.36	0.40
1:A:452:LEU:HD13	1:A:452:LEU:HA	1.91	0.40
1:A:459:GLU:H	1:A:459:GLU:HG3	1.77	0.40
1:A:1404:ALA:N	1:A:1429:LEU:H	2.20	0.40
1:B:948:LEU:HD11	1:B:994:ALA:HB1	2.04	0.40
1:B:1226:LEU:HD12	1:B:1253:HIS:CG	2.57	0.40
2:J:31:PHE:CD2	2:J:81:SER:HA	2.56	0.40
2:K:55:SER:HA	2:K:76:ARG:HH12	1.85	0.40
1:A:1364:GLY:HA2	1:A:1375:ALA:HA	2.03	0.40
1:B:911:TRP:CE3	1:B:964:VAL:HG21	2.56	0.40
1:B:1353:LEU:HD12	1:B:1388:ARG:NH2	2.36	0.40
1:B:1402:TYR:HD1	1:B:1426:MET:HG3	1.85	0.40
1:A:38:VAL:HG21	1:A:286:HIS:HB3	2.03	0.40
1:A:752:ILE:HD11	1:A:777:ASP:HA	2.02	0.40
1:B:246:ARG:HH11	1:B:246:ARG:N	2.19	0.40
1:B:400:PRO:HB3	1:B:424:ALA:N	2.36	0.40
1:B:769:TRP:NE1	1:B:801:GLN:HE22	2.20	0.40
1:B:1017:VAL:HB	1:B:1065:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1573/1869 (84%)	1531 (97%)	42 (3%)	0	100	100
1	B	1568/1869 (84%)	1526 (97%)	42 (3%)	0	100	100
2	J	199/249 (80%)	196 (98%)	3 (2%)	0	100	100
2	K	199/249 (80%)	194 (98%)	5 (2%)	0	100	100
3	I	203/236 (86%)	198 (98%)	5 (2%)	0	100	100
3	L	203/236 (86%)	199 (98%)	4 (2%)	0	100	100
All	All	3945/4708 (84%)	3844 (97%)	101 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1167/1389 (84%)	1130 (97%)	37 (3%)	34	56
1	B	1165/1389 (84%)	1124 (96%)	41 (4%)	32	54
2	J	170/203 (84%)	166 (98%)	4 (2%)	43	63
2	K	170/203 (84%)	164 (96%)	6 (4%)	32	54
3	I	185/208 (89%)	179 (97%)	6 (3%)	34	56
3	L	185/208 (89%)	176 (95%)	9 (5%)	22	47
All	All	3042/3600 (84%)	2939 (97%)	103 (3%)	33	55



All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	57	LEU
1	A	92	VAL
1	A	222	CYS
1	A	232	VAL
1	A	233	MET
1	A	314	GLN
1	A	335	VAL
1	A	362	LYS
1	A	374	ILE
1	A	422	THR
1	A	497	SER
1	A	518	VAL
1	A	522	SER
1	A	544	VAL
1	A	647	SER
1	A	660	GLN
1	A	687	VAL
1	A	708	HIS
1	A	722	ILE
1	A	747	GLU
1	A	807	VAL
1	A	819	LEU
1	A	964	VAL
1	A	988	GLU
1	A	1176	HIS
1	A	1185	LEU
1	A	1261	VAL
1	A	1281	VAL
1	A	1286	CYS
1	A	1313	THR
1	A	1328	ASP
1	A	1525	VAL
1	A	1530	THR
1	A	1544	LEU
1	A	1545	ARG
1	A	1570	LEU
1	B	9	VAL
1	B	27	ILE
1	B	57	LEU
1	B	112	SER
1	B	207	LEU

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	267	SER
1	B	307	THR
1	B	335	VAL
1	B	365	LEU
1	B	397	THR
1	B	419	GLU
1	B	466	LEU
1	B	488	LEU
1	B	497	SER
1	B	498	LEU
1	B	518	VAL
1	B	522	SER
1	B	568	VAL
1	B	589	VAL
1	B	601	VAL
1	B	708	HIS
1	B	765	VAL
1	B	807	VAL
1	B	816	VAL
1	B	823	THR
1	B	876	ARG
1	B	903	ASP
1	B	1015	THR
1	B	1154	THR
1	B	1156	ASP
1	B	1180	ILE
1	B	1233	LEU
1	B	1396	VAL
1	B	1398	ILE
1	B	1405	THR
1	B	1454	ASP
1	B	1490	THR
1	B	1530	THR
1	B	1555	THR
1	B	1561	ILE
2	J	61	THR
2	J	84	TYR
2	J	158	THR
2	J	211	ASN
2	K	18	ARG
2	K	53	ILE

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Mol	Chain	Res	Type
2	K	61	THR
2	K	101	THR
2	K	167	THR
2	K	202	ILE
3	I	23	SER
3	I	37	ILE
3	I	68	LEU
3	I	106	VAL
3	I	128	ILE
3	I	200	THR
3	L	20	MET
3	L	22	GLN
3	L	37	ILE
3	L	68	LEU
3	L	82	ARG
3	L	90	THR
3	L	112	SER
3	L	115	THR
3	L	160	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	HIS
1	A	554	GLN
1	A	696	ASN
1	B	136	ASN
1	B	304	ASN
1	B	310	ASN
1	B	338	HIS
1	B	447	ASN
1	B	877	HIS
1	B	910	GLN
2	K	178	GLN
3	I	52	ASN
3	L	52	ASN
3	L	211	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4HH	B	1538	1	22,26,27	1.22	1 (4%)	27,35,37	0.95	1 (3%)
1	4HH	A	1538	1	22,26,27	1.22	1 (4%)	27,35,37	0.95	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4HH	B	1538	1	-	18/33/35/37	-
1	4HH	A	1538	1	-	17/33/35/37	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1538	4HH	CL3-NN	2.37	1.39	1.33
1	A	1538	4HH	CL3-NN	2.33	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1538	4HH	O1P-P-O2P	2.23	122.84	112.44
1	B	1538	4HH	O1P-P-O2P	2.23	122.80	112.44
1	A	1538	4HH	CO-CP-CQ	-2.03	109.02	112.39

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1538	4HH	CA-CB-OG-P
1	A	1538	4HH	CB-OG-P-O1P
1	A	1538	4HH	CB-OG-P-O3P
1	A	1538	4HH	O3P-CJ-CK-CL1
1	A	1538	4HH	O3P-CJ-CK-CL2
1	A	1538	4HH	O3P-CJ-CK-CM
1	A	1538	4HH	CM-CL3-NN-CO
1	A	1538	4HH	CJ-O3P-P-O1P
1	A	1538	4HH	NN-CO-CP-CQ
1	B	1538	4HH	CB-OG-P-O2P
1	B	1538	4HH	O3P-CJ-CK-CL1
1	B	1538	4HH	O3P-CJ-CK-CL2
1	B	1538	4HH	O3P-CJ-CK-CM
1	B	1538	4HH	CJ-CK-CM-CL3
1	B	1538	4HH	CJ-CK-CM-OM
1	B	1538	4HH	CL1-CK-CM-CL3
1	B	1538	4HH	CL1-CK-CM-OM
1	B	1538	4HH	CL2-CK-CM-CL3
1	B	1538	4HH	CL2-CK-CM-OM
1	B	1538	4HH	CM-CL3-NN-CO
1	B	1538	4HH	CP-CQ-NR-CS
1	A	1538	4HH	ON-CL3-NN-CO
1	B	1538	4HH	ON-CL3-NN-CO
1	B	1538	4HH	OR-CQ-NR-CS
1	A	1538	4HH	CO-CP-CQ-OR
1	A	1538	4HH	CO-CP-CQ-NR
1	B	1538	4HH	CA-CB-OG-P
1	A	1538	4HH	ON-CL3-CM-OM
1	B	1538	4HH	CB-OG-P-O3P
1	A	1538	4HH	CL2-CK-CM-CL3
1	A	1538	4HH	CK-CJ-O3P-P
1	B	1538	4HH	CK-CJ-O3P-P
1	A	1538	4HH	CJ-CK-CM-CL3
1	A	1538	4HH	NN-CL3-CM-OM
1	B	1538	4HH	NN-CL3-CM-OM

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1538	4HH	2	0
1	A	1538	4HH	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

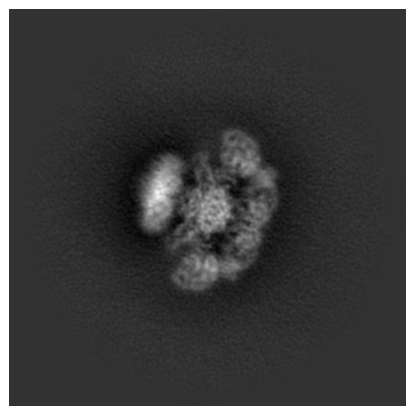
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71497. These allow visual inspection of the internal detail of the map and identification of artifacts.

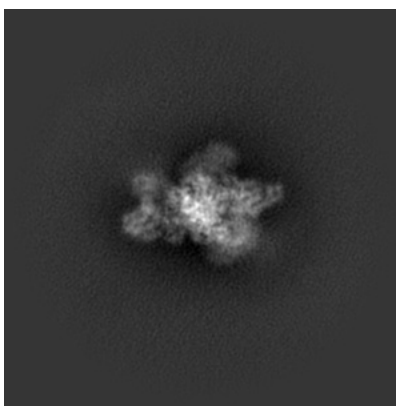
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

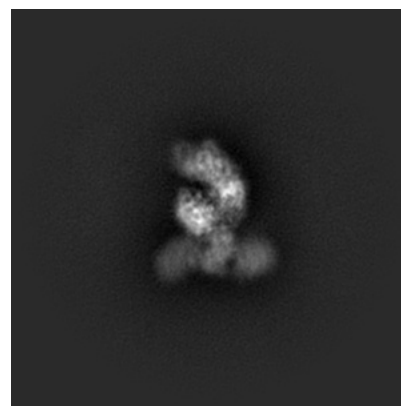
#### 6.1.1 Primary map



X

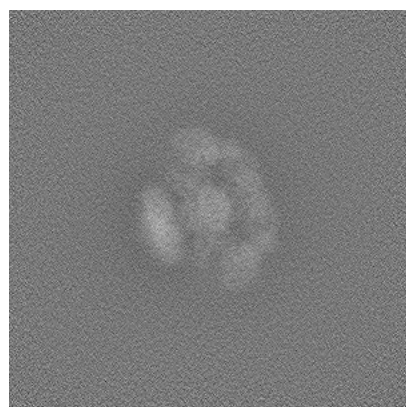


Y

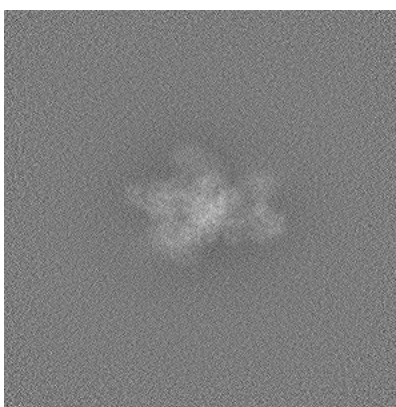


Z

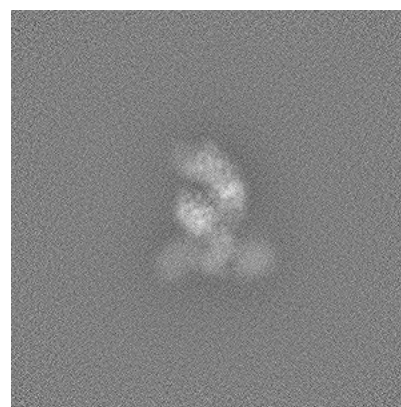
#### 6.1.2 Raw map



X



Y

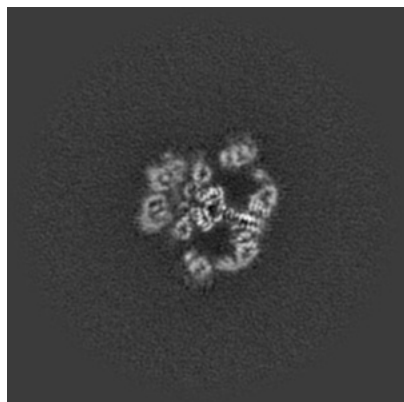


Z

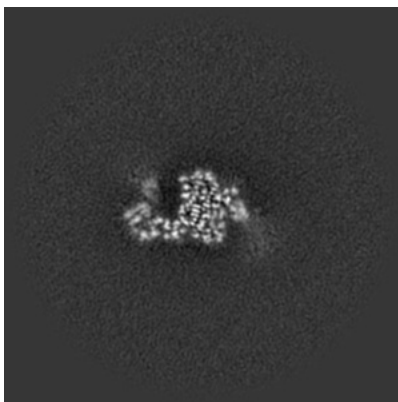
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

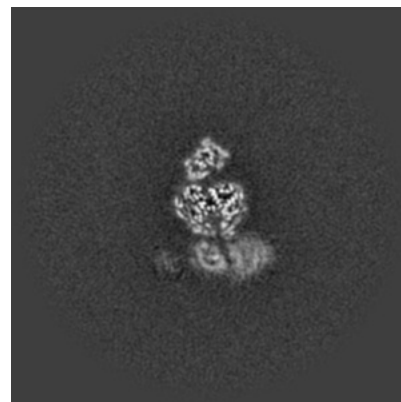
### 6.2.1 Primary map



X Index: 300

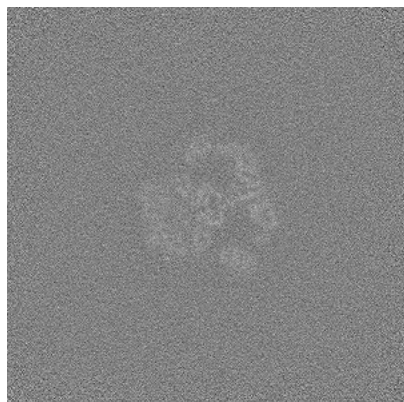


Y Index: 300

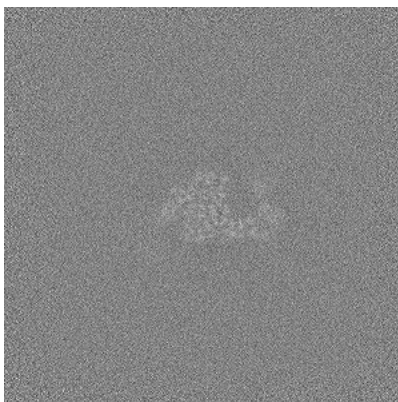


Z Index: 300

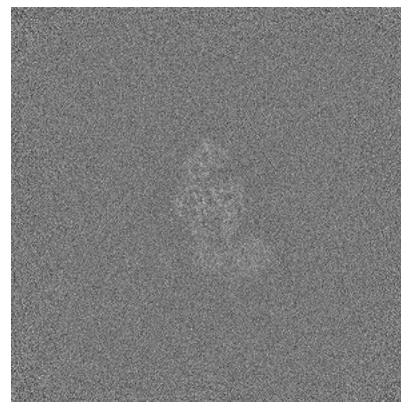
### 6.2.2 Raw map



X Index: 300



Y Index: 300



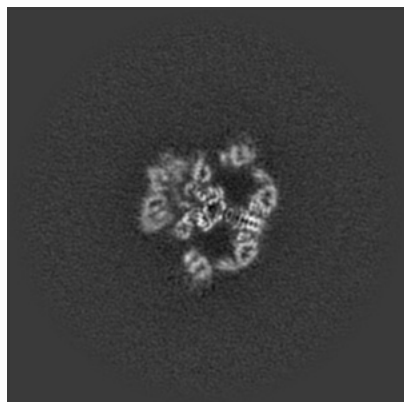
Z Index: 300

The images above show central slices of the map in three orthogonal directions.

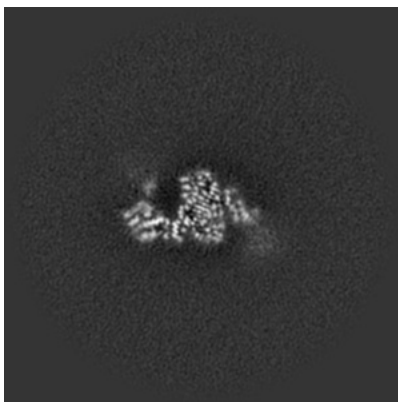


## 6.3 Largest variance slices [i](#)

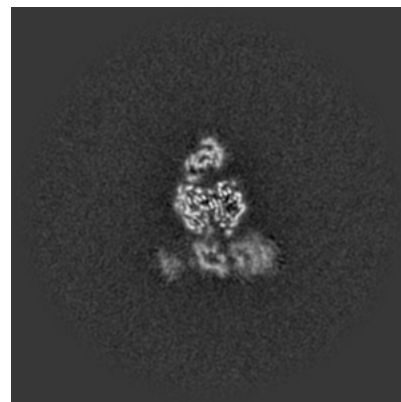
### 6.3.1 Primary map



X Index: 298

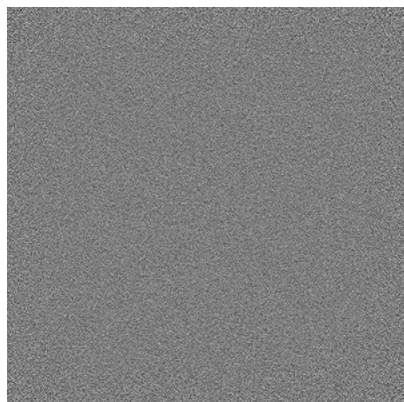


Y Index: 297

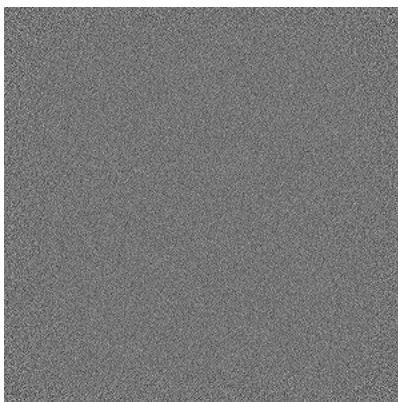


Z Index: 306

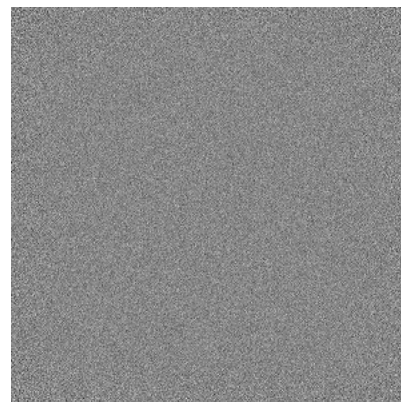
### 6.3.2 Raw map



X Index: 0



Y Index: 0

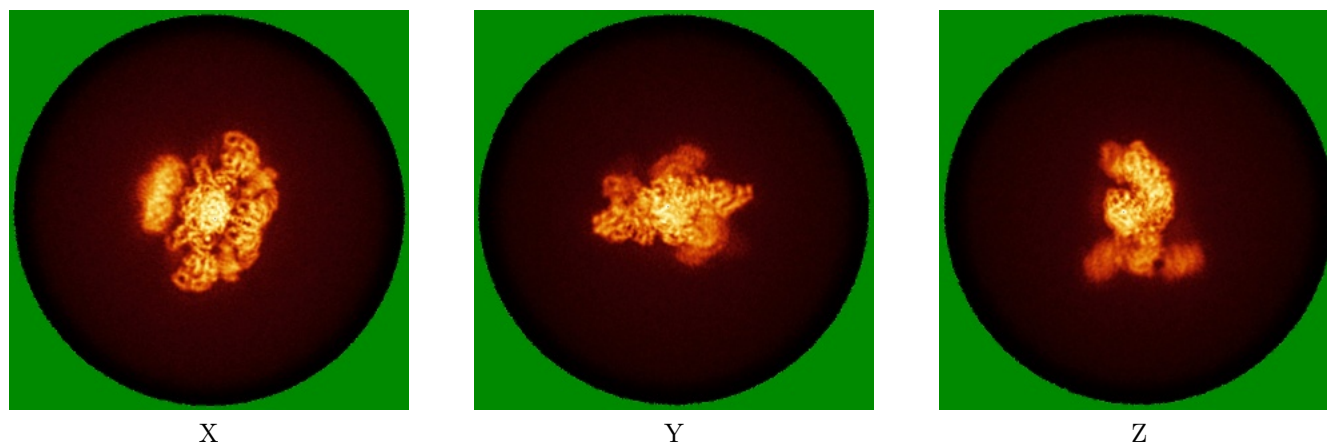


Z Index: 0

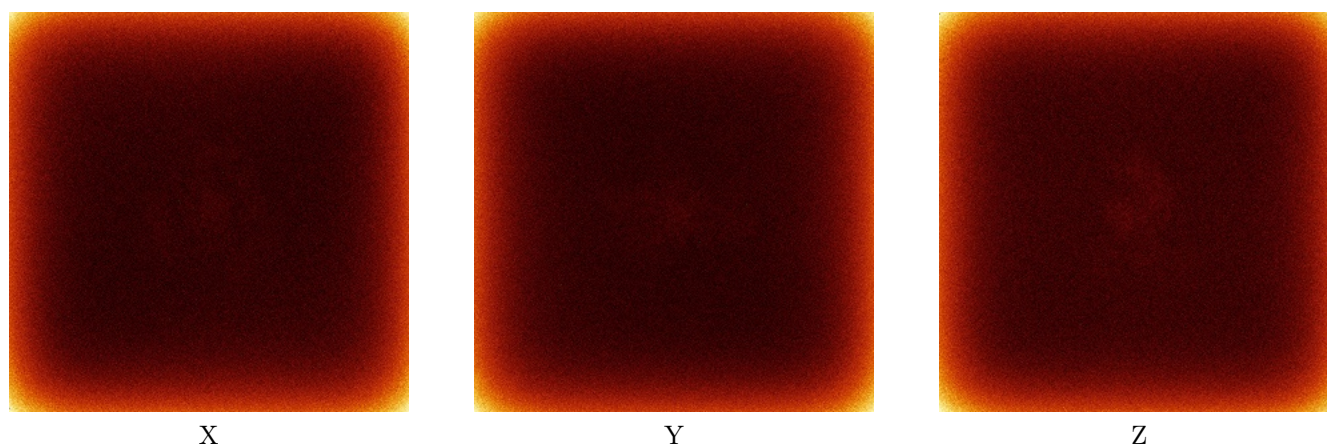
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

This section was not generated.

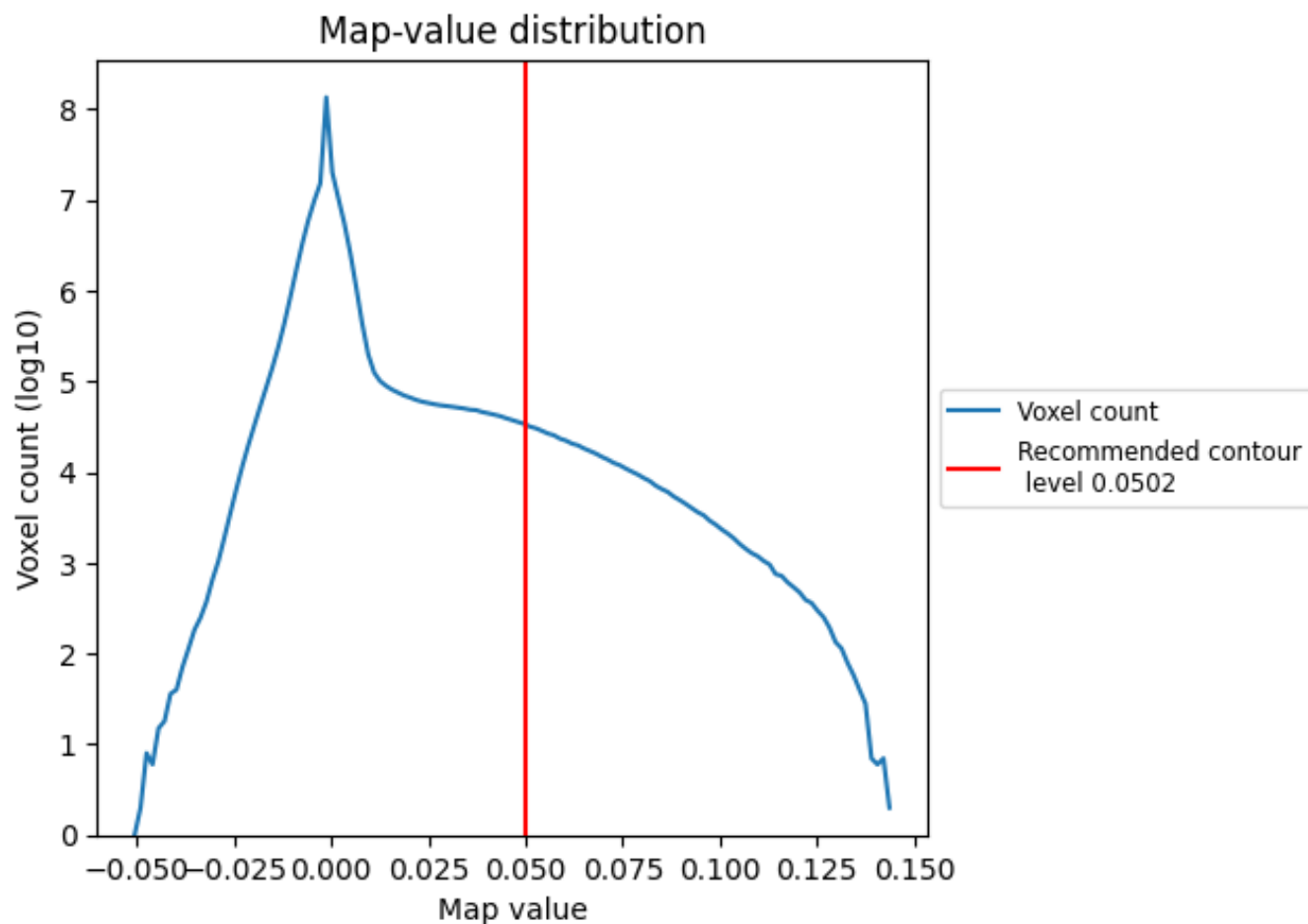
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

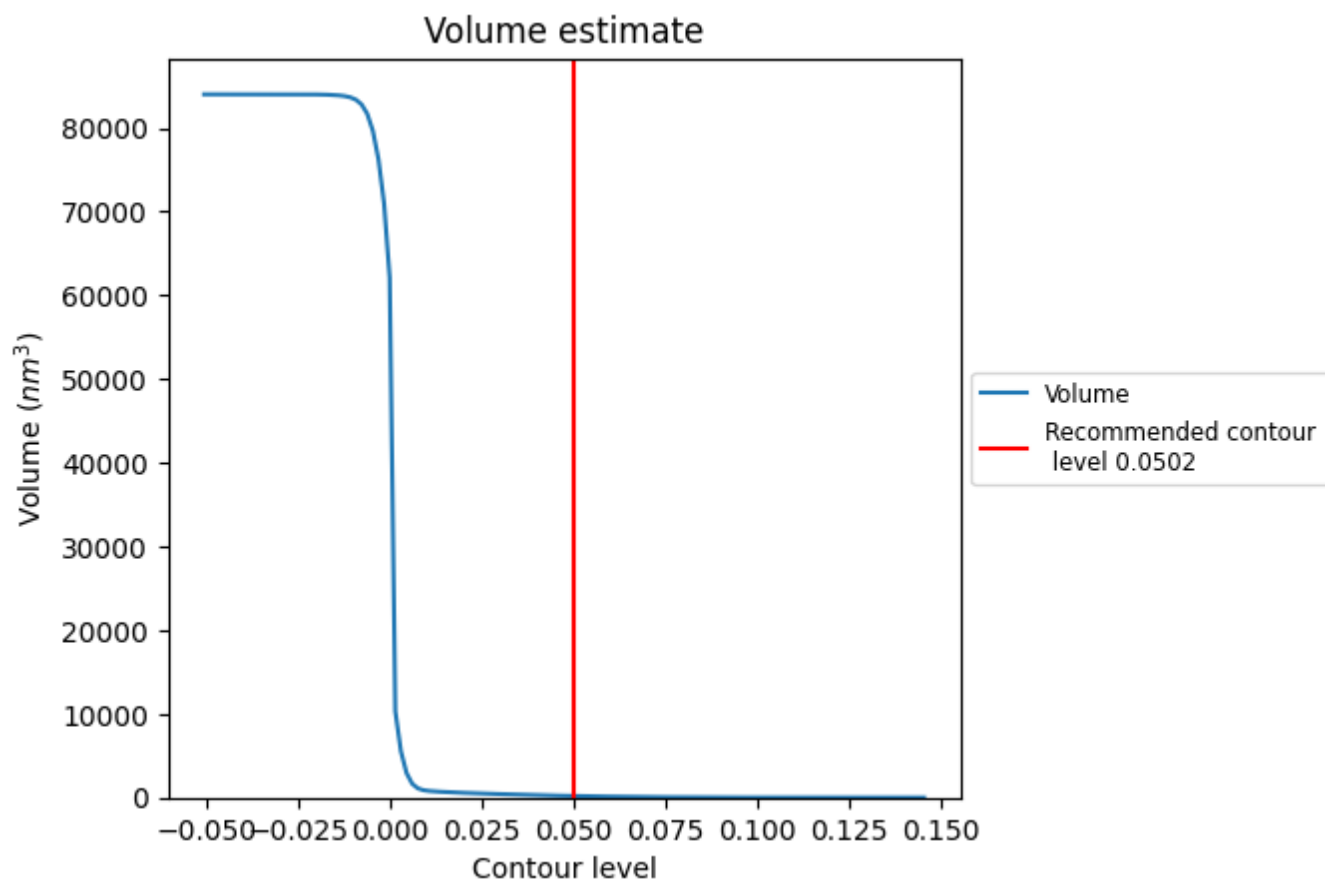
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

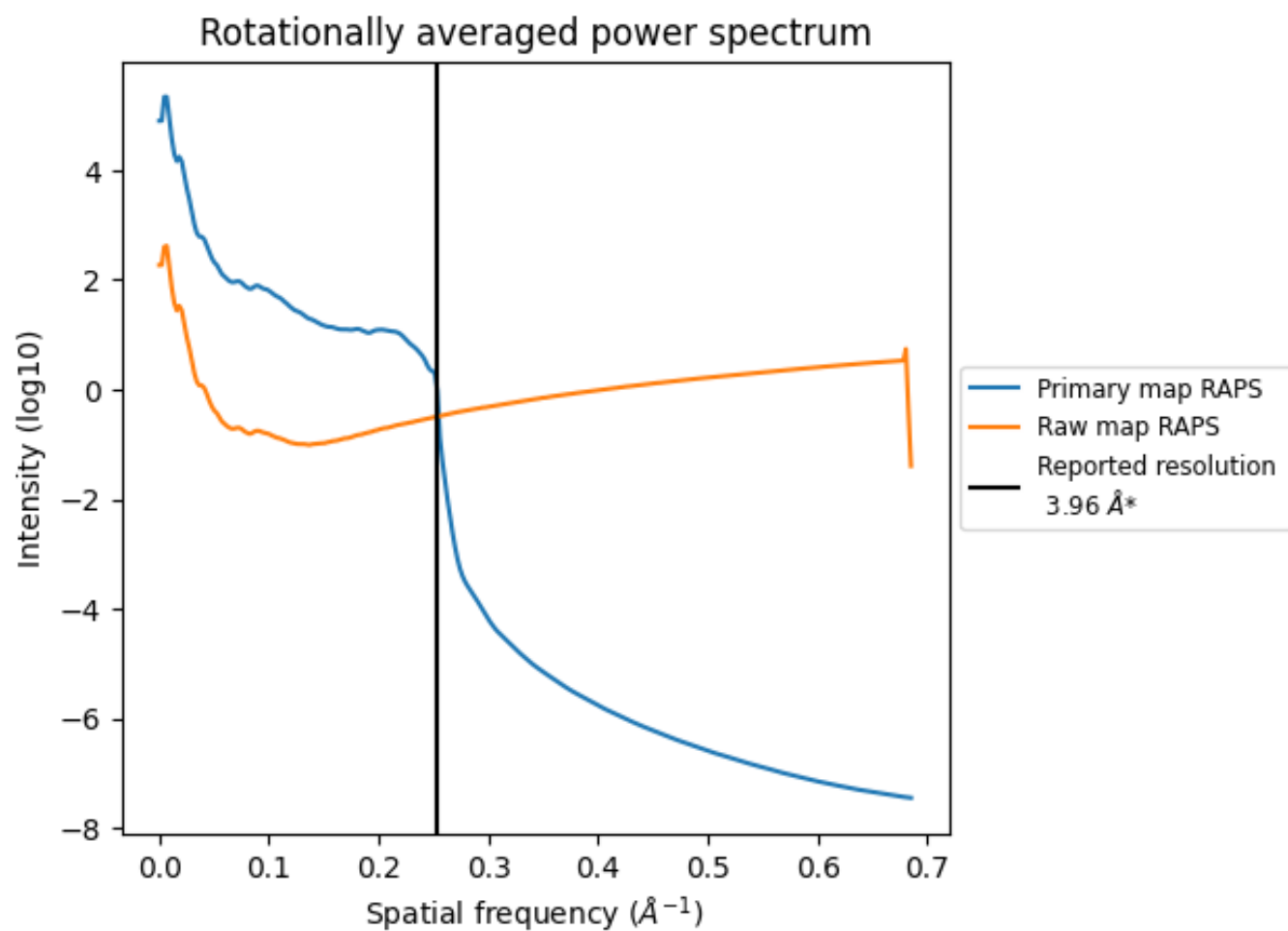
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm<sup>3</sup>; this corresponds to an approximate mass of 165 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

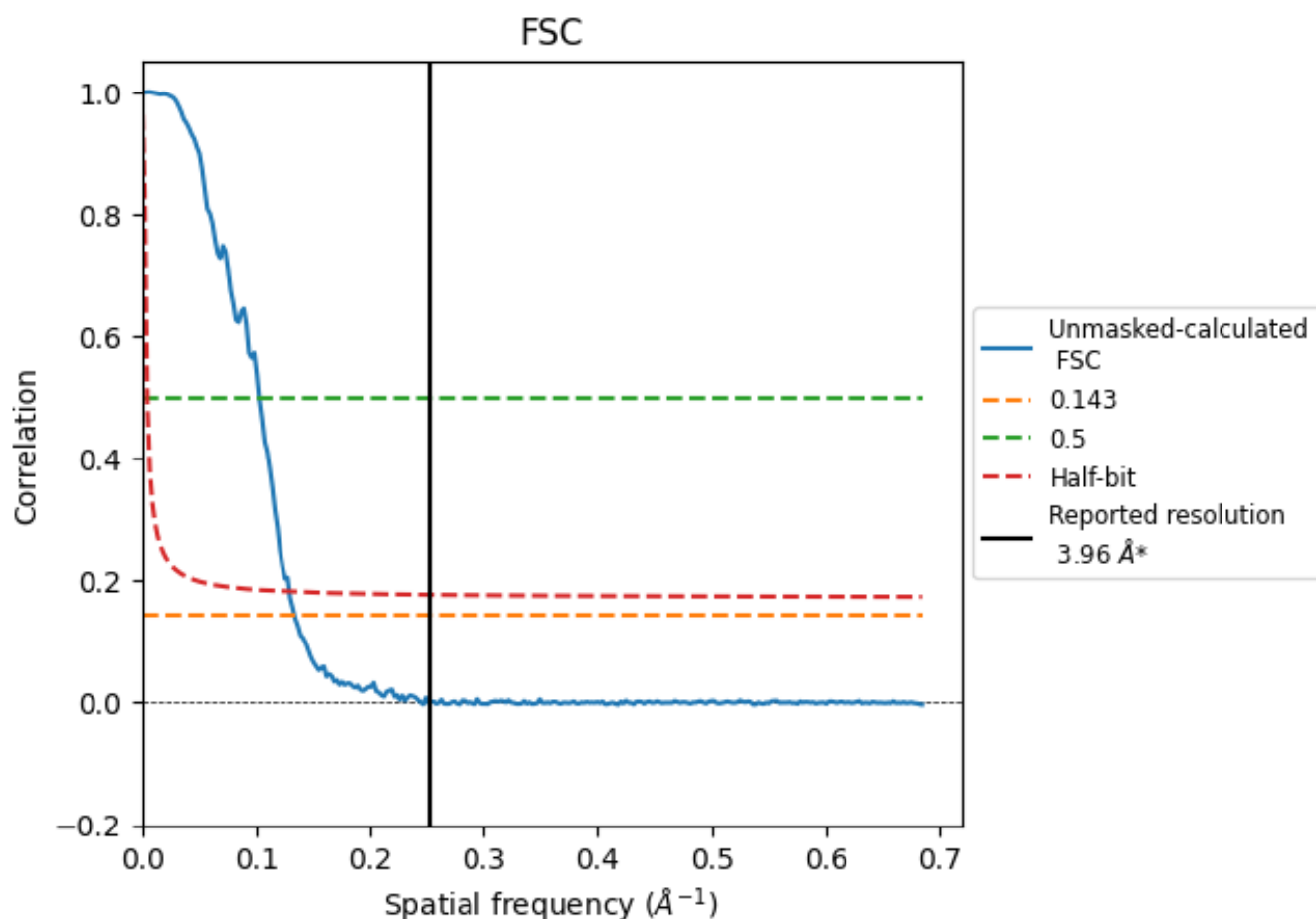


\*Reported resolution corresponds to spatial frequency of 0.253  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.253  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

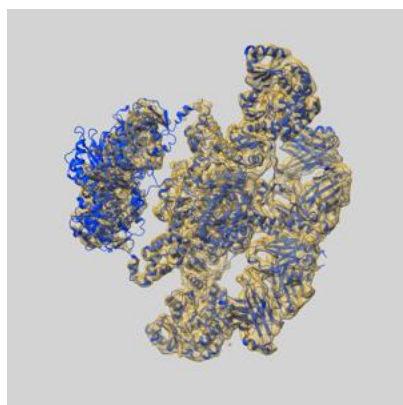
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.46	9.76	7.73

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.46 differs from the reported value 3.96 by more than 10 %

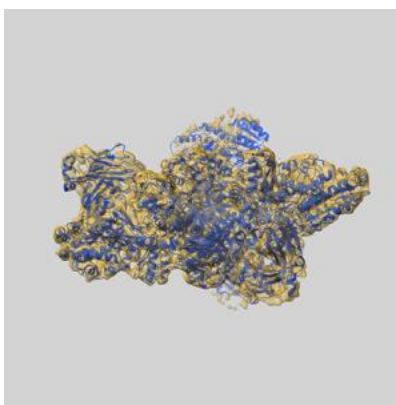
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71497 and PDB model 9PC6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

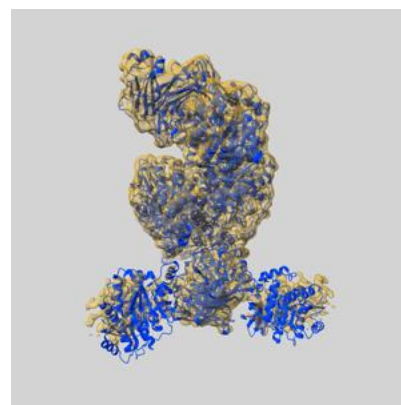
### 9.1 Map-model overlay [i](#)



X



Y

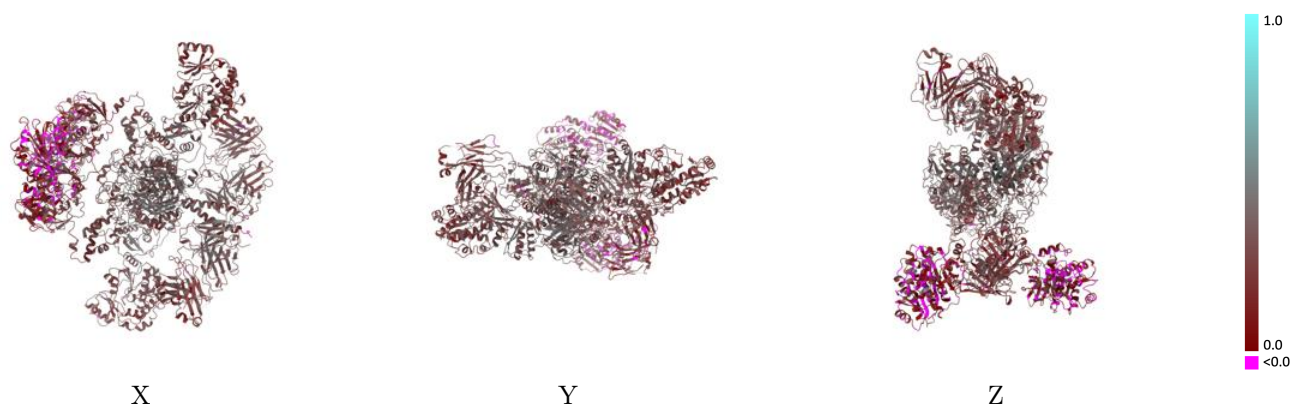


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0502 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

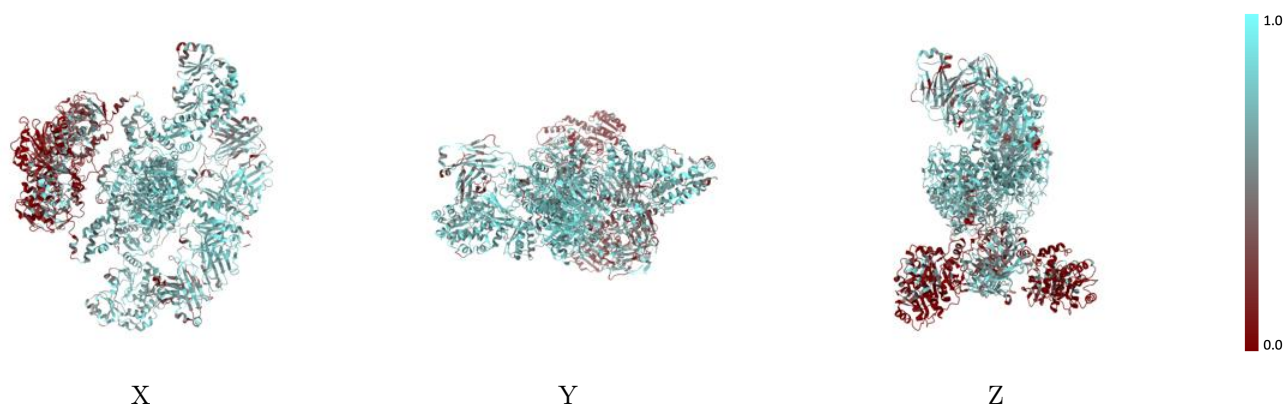


## 9.2 Q-score mapped to coordinate model [i](#)



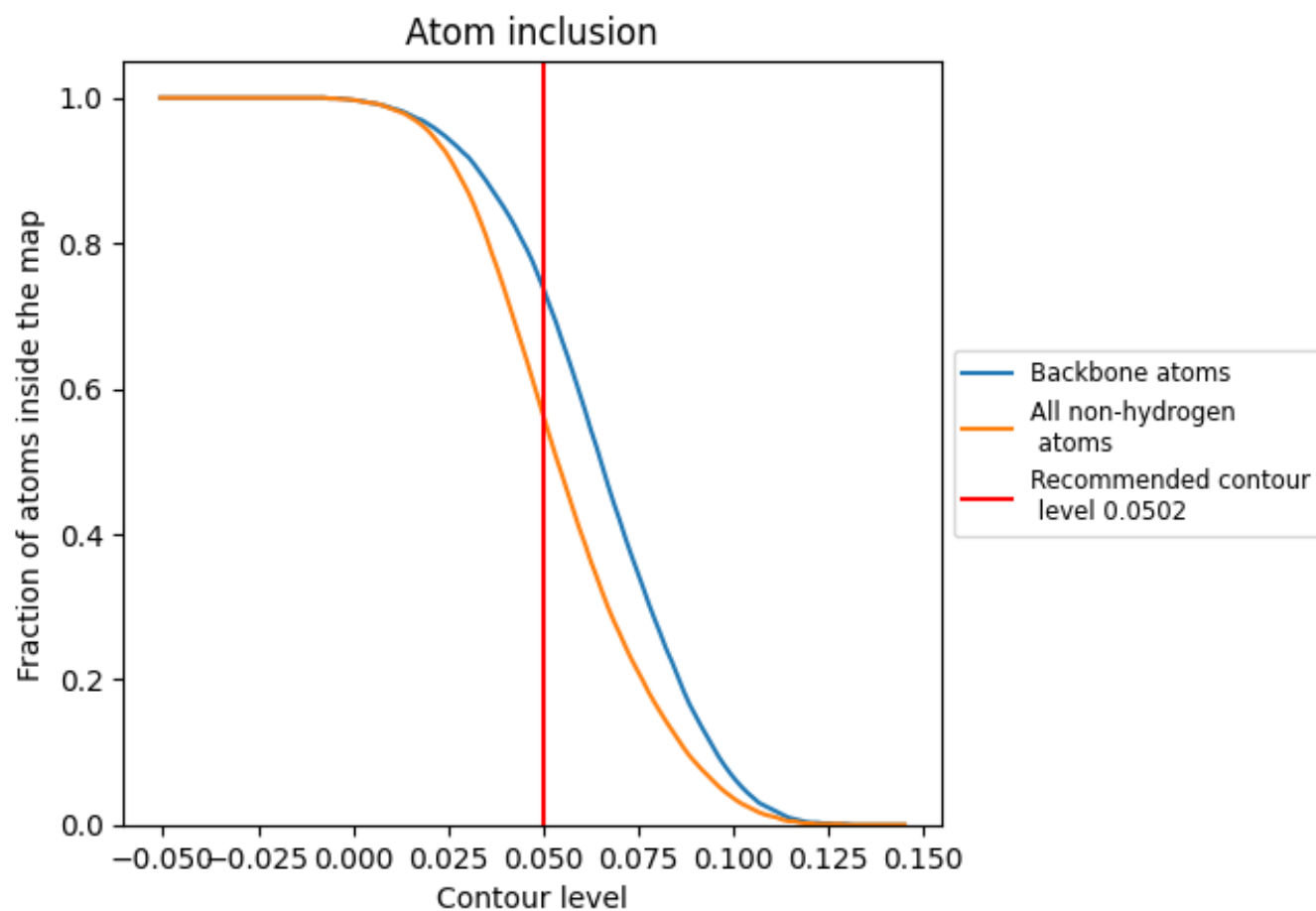
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0502).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0502) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5610</div>	<div><div></div>0.2850</div>
A	<div><div></div>0.5280</div>	<div><div></div>0.2720</div>
B	<div><div></div>0.5420</div>	<div><div></div>0.2780</div>
I	<div><div></div>0.6760</div>	<div><div></div>0.3180</div>
J	<div><div></div>0.6450</div>	<div><div></div>0.3180</div>
K	<div><div></div>0.6450</div>	<div><div></div>0.3280</div>
L	<div><div></div>0.6680</div>	<div><div></div>0.3280</div>

1.0

0.0

<0.0